Dipartimento di Scienze Matematiche G. L. Lagrange

A PDE approach to centroidal tessellations of domains

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Outline

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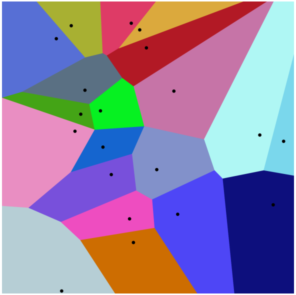
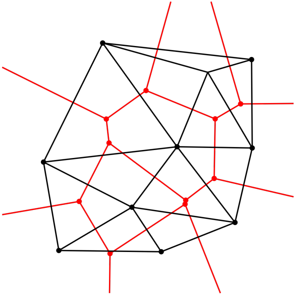
Voronoi diagrams

- A Voronoi diagram is a partition of a plane into regions close to each of a given set of objects. In the simplest case, these objects are just finitely many points in the plane (called generators).
- For each seed there is a corresponding region, called a Voronoi cell, consisting of all points of the plane closer to that seed than to any other.
- The Voronoi diagram of a set of points is dual to its Delaunay triangulation.



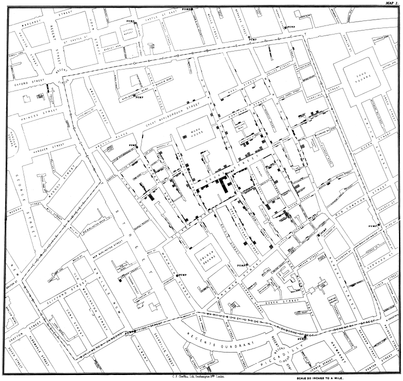


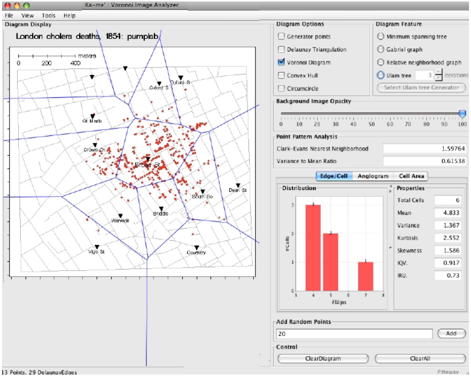
Voronoi diagrams have been used in many fields of science

- In biology, Voronoi diagrams are used to model a number of different biological structures, including cells and bone microarchitecture.
- In hydrology, Voronoi diagrams are used to calculate the rainfall of an area, based on a series of point measurements.
- In ecology, Voronoi diagrams are used to study the growth patterns of forests and fire growth predictions.
- In astrophysics, Voronoi diagrams are used to generate adaptative smoothing zones on images, adding signal fluxes on
- In epidemiology, Voronoi diagrams can be used to correlate sources of infections in epidemics.
- And many others...

My personal favourite: one of the early applications of Voronoi diagrams was implemented by John Snow to study the 1854 Broad Street cholera outbreak in Soho, England. He showed the correlation between residential areas on the map of Central London whose residents had been using a specific water pump, and the areas with the most deaths due to the outbreak.

Even though, I see some troubles..





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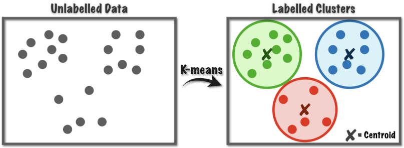
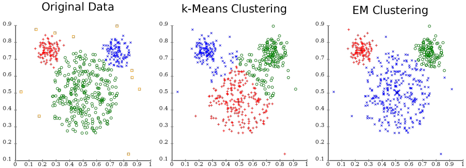
Clustering and K-means

k-means clustering is a method of vector quantization, originally from signal processing, that aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean (cluster centers or cluster centroid), serving as a prototype of the cluster.

This results in a partitioning of the data space into Voronoi cells.



Different cluster analysis results on "mouse" data set:



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The K-means problem and the Lloyd algorithm

Ω is a bounded subset of $\mathbb{R}^d$ and ρ is a density function supported in Ω, i.e., $\rho \geq 0$ and $\int_\Omega \rho dx = 1$, representing the distribution of the points of a given data set $\mathcal{X}$.

The K-means problem aims to minimize the functional

$$\mathcal{I}(y_1, \dots, y_k) = \sum_{k=1}^{K} \int_{V(y_k)} |x - y_k|^2 \rho(x) dx, \quad (1)$$

$$\text{where} \quad V(y_k) = \{x \in \mathbb{R}^d : |x - y_k| = \min_{j=1,\dots,K} |x - y_j|\}. \quad (2)$$

Where the minimum of the functional $\mathcal{I}$ provides a clusterization of the data set, i.e., a repartition of $\mathcal{X}$ into K disjoint clusters $V(y_k)$ such that each data point belongs to the cluster with the nearest centroid y_k.

This property can be expressed in the elegant terminology of the *centroidal Voronoi tessellations*.

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Voronoi tassellation

Given a set of generators $\{y_k\}_{k=1}^K$, $y_k \in \overline{\Omega}$, the Voronoi region corresponding to y_k is defined as in (2) (the point of $V(y_k) \cap V(y_j)$ are assigned to the diagram with the smaller index). The family $\{V(y_k)\}_{k=1}^K$ determines a tessellation of Ω, i.e. $V(y_i)^{\mathrm{o}} \cap V(y_j)^{\mathrm{o}} = \emptyset$ for $i \neq j$ and $\cup_{i=1}^K V(y_i) = \overline{\Omega}$.

Definition

A Voronoi tessellation $\{V(y_k)\}_{k=1}^K$ of Ω is said to be a centroidal Voronoi tessellation (CVT in short) if, for each $k = 1, \ldots, K$, the generator y_k of $V(y_k)$ coincides with the centroid of $V(y_k)$, i.e.

$$y_k = \frac{\int_{V(y_k)} s\rho(s)ds}{\int_{V(y_k)} \rho(s)ds}.$$

Since Ω is bounded and $\mathcal{I}$ is continuous, a global minimum of the functional exists; but, since $\mathcal{I}$ is in general non convex, local minimums may also exist. It is possible to show that:

$$\text{critical points of } \mathcal{I} \text{ correspond to CVTs of } \Omega. \tag{3}$$

Critical points of $\mathcal{I}$ can be computed via the Lloyd algorithm, a simple two steps iterative procedure.

The Lloyd algorithm

Starting from an arbitrary initial set of generators, at each iteration the following two steps are performed

1. construct the Voronoi tessellation $\{V(y_i)\}_{i=1}^{K}$;
2. take the centroids of $\{V(y_i)\}_{i=1}^{K}$ as the new set of generators.

The procedure is repeated until an appropriate stopping criterion is met. At each iteration, the objective function $\mathcal{I}$ decreases and the algorithm converges to a (local) minimum of (1).

Relationship with Mean Field Games theory

The problem can be seen also as a equilibrium point for a system of partial differential equations arising in the the theory of Mean Field Games. [Aquilanti et al. '21]

If we consider the multi-population MFG system, for $k = 1, \dots, K$

$$\begin{cases} -\varepsilon\Delta u_{k,\varepsilon} + \frac{1}{2}|Du_{k,\varepsilon}|^2 + \lambda_{k,\varepsilon} = \frac{\varepsilon^2}{2}(x-\mu_{k,\varepsilon})^t(\Sigma_{k,\varepsilon}^{-1})^t\Sigma_{k,\varepsilon}^{-1}(x-\mu_{k,\varepsilon}), & x \in \mathbb{R}^d, \\ \varepsilon\Delta m_{k,\varepsilon} + \operatorname{div}(m_{k,\varepsilon}Du_{k,\varepsilon}) = 0, & x \in \mathbb{R}^d, \\ \alpha_{k,\varepsilon} = \int_{\mathbb{R}^d}\gamma_{k,\varepsilon}(x)\rho(x)dx, \\ m_{k,\varepsilon} \geq 0,\ \int_{\mathbb{R}^d} m_{k,\varepsilon}dx = 1,\ u_{k,\varepsilon}(\mu_{k,\varepsilon}) = 0, \end{cases} \tag{4}$$

$$\gamma_{k,\varepsilon}(x) = \frac{\alpha_{k,\varepsilon}m_{k,\varepsilon}(x)}{\sum_{j=1}^K \alpha_{j,\varepsilon}m_{j,\varepsilon}(x)}, \quad \mu_{k,\varepsilon} = \frac{\int_{\mathbb{R}^d} x\gamma_{k,\varepsilon}(x)\rho(x)dx}{\int_{\mathbb{R}^d}\gamma_{k,\varepsilon}(x)\rho(x)dx}, \tag{5}$$

$$\Sigma_{k,\varepsilon} = \frac{\int_{\mathbb{R}^d}(x-\mu_{k,\varepsilon})(x-\mu_{k,\varepsilon})^t\gamma_{k,\varepsilon}(x)\rho(x)dx}{\int_{\mathbb{R}^d}\gamma_{k,\varepsilon}(x)\rho(x)dx}. \tag{6}$$

More precisely, a solution of (4) is given by a family of quadruples $(u_{k,\varepsilon}, \lambda_{k,\varepsilon}, m_{k,\varepsilon}, \alpha_{k,\varepsilon})$, $k = 1, \dots, K$, with

$$\begin{aligned} u_{k,\varepsilon}(x) &= \frac{\varepsilon}{2}(x-\mu_{k,\varepsilon})^t \Sigma_{k,\varepsilon}^{-1}(x-\mu_{k,\varepsilon}), \quad \lambda_{k,\varepsilon} = \varepsilon^2 \mathrm{Tr}(\Sigma_{k,\varepsilon}^{-1}), \\ m_{k,\varepsilon}(x) &= \mathcal{N}(x;\mu_{k,\varepsilon},\Sigma_{k,\varepsilon}) = C_k e^{-\frac{u_k(x)}{\varepsilon}}, \\ \alpha_{k,\varepsilon} &= \int_{\mathbb{R}^d} \gamma_{k,\varepsilon}(x)\rho(x)dx, \end{aligned} \tag{7}$$

and the corresponding parameters $(\alpha_{k,\varepsilon}, \mu_{k,\varepsilon}, \Sigma_{k,\varepsilon})$, $k = 1, \dots, K$, are an equilibrium. Note that in general the solution of (4) is not unique.

In cluster analysis, the responsibilities can be used to assign a point to the class with the highest $\gamma_{k,\varepsilon}$, i.e. the data set is divided into the disjoint subsets

$$S^k_{u,\varepsilon} = \{x \in \mathbb{R}^d : \gamma_{k,\varepsilon}(x) = \max_{j=1,\dots,K} \gamma_{j,\varepsilon}(x)\}.$$

Taking into account the definition of $\gamma_{k,\varepsilon}$ and $m_{k,\varepsilon}$, we see that the clusters $S^k_{u,\varepsilon}$ can be equivalently defined as

$$S^k_{u,\varepsilon} = \{x \in \mathbb{R}^d : u_{k,\varepsilon}(x) = \min_{j=1,\dots,K} u_{j,\varepsilon}(x)\}. \tag{8}$$

A system of Hamilton-Jacobi equations for the K-means problem

- In order to deduce a PDE characterization for centroidal Voronoi tessellations, we interpret the convergence of maximum likelihood functional to the K means functional in term of the limit in the MFG system.
- Assuming that $\Sigma_k = \sigma I$ and passing to the limit for $\varepsilon, \sigma \to 0^+$ in such a way that $\varepsilon/\sigma^2 \to 1$, we observe that the responsibility $\gamma_{k,\varepsilon}$ converges to the characteristic function of the set where $\alpha_k m_k$ is maximum with respect to $\alpha_j m_j$, $j = 1, \dots, K$ or, equivalently, where u_k is minimum with respect to u_j.
- Hence, we formally obtain that (4) converges to the first order multi-population MFG system

$$\begin{cases} \frac{1}{2}|Du_k|^2 + \lambda_k = \frac{1}{2}|x-\mu_k|^2, & x \in \mathbb{R}^d, \\ \operatorname{div}(m_k Du_k(x)) = 0, & x \in \mathbb{R}^d, \\ \alpha_k = \int_{\mathbb{R}^d} \mathbb{1}_{S_u^k}(x)\rho(x)dx, & \\ m_k \geq 0,\ \int_{\mathbb{R}^d} m_k(x)dx = 1, u_k(\mu_k) = 0, & \end{cases} \tag{9}$$

for $k = 1, \dots, K$, with

$$S_u^k = \{x \in \mathbb{R}^d : u_k(x) = \min_{j=1,\dots,K} u_j(x)\}, \tag{10}$$

$$\mu_k = \frac{\int_{\mathbb{R}^d} x \mathbb{1}_{S_u^k}(x)\rho(x)dx}{\int_{\mathbb{R}^d} \mathbb{1}_{S_u^k}(x)\rho(x)dx}. \tag{11}$$

Recalling that the unique viscosity solution of the problem

$$\begin{cases} |Du| = 1 \quad x \in \mathbb{R}^d, \\ u(\mu) = 0, \end{cases}$$

is given by $u(x) = |x - \mu|$, we can write the following simplified version of (9)

$$\begin{cases} |Du_k| = 1 \quad x \in \mathbb{R}^d, \\ u_k(\mu_k) = 0, \\ S_u^k = \{x \in \mathbb{R}^d : \; u_k(x) = \min_{j=1,\dots,K} u_j(x)\}, \\ \mu_k = \dfrac{\int_{\mathbb{R}^d} x \mathbb{1}_{S_u^k}(x)\rho(x)dx}{\int_{\mathbb{R}^d} \mathbb{1}_{S_u^k}(x)\rho(x)dx} \end{cases} \tag{12}$$

for $k = 1, \dots, K$, which is a system of K HJ equations coupled through the sets S_u^k.

- For each k, the first two conditions in (12) imply that u_k is the the Euclidean distance from μ_k,
- the third condition determine the Voronoi diagram corresponding to the generator μ_k,
- the last condition entails μ_k being the centroid of S_u^k.

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We now show that the multi-population MFG system characterizes critical points of the functional (1) or, equivalently, CVTs of the set Ω.

Proposition

We have:

(i) *Let $(y_1, \dots, y_K)$ be a critical point of the functional $\mathcal{I}$ in (1) with Voronoi diagrams $V(y_k)$. Then, there exists a solution of the MFG system such that $\mu_k = y_k$ and $S_u^k = V(y_k)$.*

(ii) *Given a solution $u = (u_1, \dots, u_K)$ of the MFG system, then $(\mu_1, \dots, \mu_K)$ is a critical point of $\mathcal{I}$ with Voronoi diagrams $V(y_k) = S_u^k$.*

The previous result can be restated in the terminology of the Voronoi tessellation, saying that a solution of the MFG system determine a CVT and vice versa.

Finally, we have the following existence result the MFG system.

Theorem

Let ρ be a positive and smooth density function defined on a smooth bounded set Ω. Then, there exists a solution u to the MFG system. Moreover, any limit point of the Lloyd algorithm determine a solution of MFG system.

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A PDE algorithm for the K-means problem

We describe and test a method for the K-means problem obtained by combining the numerical approximation of the system (12) with the Lloyd algorithm.

- We introduce a regular triangulation of Ω, the support of ρ, given by a collection of N disjoint triangles $\mathcal{T} := \{T_i\}_{i=1,\dots,N}$.
- We denote with Δx the maximal area of the triangles, i.e. $\max_{i=1,\dots,N} |T_i| < \Delta x$, and we assume that $\Omega \subseteq \bigcup_1^N T_i \approx \Omega$.
- We denotes with $\mathcal{G} := \{X_i\}_{i=1,\dots,N}$ the set of the centroids of the triangles T_i and, for a piecewise linear function $U : \mathcal{G} \to \mathbb{R}$, we set $U_i := U(X_i)$.
- For the approximation of the HJ equation in (12), we consider the semi-Lagrangian monotone scheme

$$G_i(U) = \min_{a \in B(0,1)} \{\mathbb{I}[U](X_i - ha) + h\},$$

where h is a fictitious-time parameter (generally taken of order $O(\sqrt{\Delta x})$, and $\mathbb{I}$ a standard linear interpolation operator on the simplices of the triangulation.

Our algorithm is a two steps iterative procedure. Starting from an arbitrary assignment $\mu^{(0)} = (\mu^{(0),1}, \ldots, \mu^{(0),K})$ for the centroids, we iterate

(i) For $k = 1, \ldots, K$ and $j_k = \text{argmin}_{i=1,\ldots,N} |X_i - \mu^{(n),k}|$, solve the problem

$$\begin{cases} G_i(U^{(n),k}) = 1, \quad i = 1, ..., N, \\ U^{(n),k}_{j_k} = 0, \end{cases} \tag{13}$$

(recall that $U^{(n),k}_{j_k}$ denotes the value at the n-th iteration of the approximate solution of the k-th equation at point X_{j_k}), and define

$$\mathcal{S}^{(n+1),k} = \bigcup \left\{ T_i : \ i \text{ is s.t. } U^{(n),k}_i = \min_{j=1,\ldots,K} U^{(n),j}_i \right\}.$$

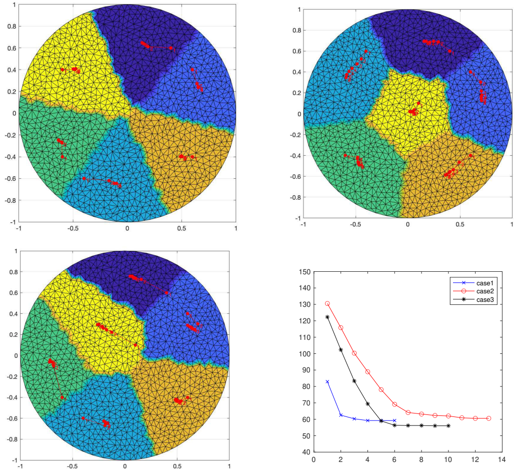
(ii) Compute the new centroids points

$$\mu^{(n+1),k} = \frac{\sum_{T_i \in \mathcal{S}^{(n+1),k}} X_i |T_i| \rho(X_i)}{\sum_{T_i \in \mathcal{S}^{(n+1),k}} |T_i| \rho(X_i)}. \tag{14}$$

We iterate these two steps till meeting a stopping criterion as

$$\max_k \{ |\mu^{(n+1),k} - \mu^{(n),k}| \} < \varepsilon.$$

Test 1 - Centroidal Voronoi tessellation of a circle.



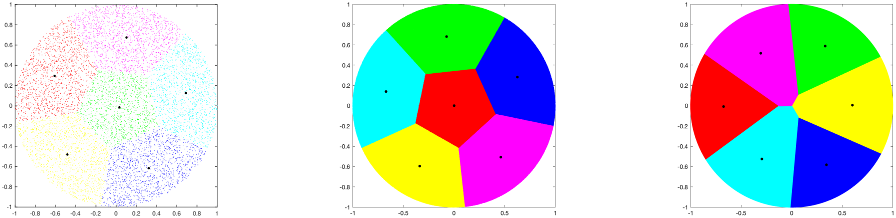
$\Omega := B(0,1)$, 6 cells, ρ uniformly distributed (i.e. $\rho(x) = 1/|\Omega|$), $\Delta x = 0.004$ and $\varepsilon = \Delta x/10$.

Performances, CPU time and comparison with sampled-based standard algorithms.

In this Test 1, with a $\Delta x = 0.004$, we reached the approximated solution after 6, 13, and 10 iterations, with the use of the *CPU* time of 78, 89, and 82 seconds depending on the initial guess of the centroids.

To compare our results with other clustering techniques we show the results obtained by the K-means++ algorithm which is, as our proposal, based on the Lloyd algorithm.

In Figure below we show the results of the K-means++ algorithm with a sample set of 10^4, $5 \cdot 10^6$, and 10^7 points for which we obtain the solution after 0.085, 28.7 and 214 seconds.



Test 2. A different domain.

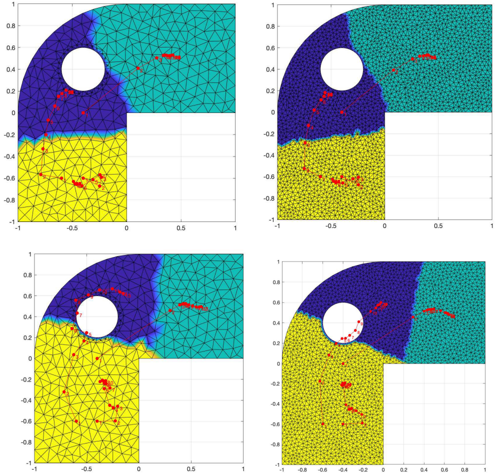


Figure: Above: uniformly distributed ρ, left: $\Delta x = 0.01$, right: $\Delta x = 0.001$. Bottom: ρ is a multivariate normal distribution around $[0.5, 0.5]$, left: $\Delta x = 0.01$; right: $\Delta x = 0.001$.

Geodesic Voronoi tessellations and HJ equations

Motivated by the relation between MFGs and CVT in the Euclidean case, we introduce a system of HJ equations which characterize CVT for a general class of convex metrics.

Consider a set-valued map $x \mapsto C(x) \subset \mathbb{R}^d$ and assume that

(H1) for each $x \in \mathbb{R}^d$, $C(x)$ is a compact, convex set and $0 \in C(x)$;

(H2) there exists $L > 0$ such that $d_{\mathcal{H}}(C(x), C(y)) \leq L|x - y|$, for all $x, y \in \mathbb{R}^d$;

(H3) there exists $\delta > 0$ such $B(0, \delta) \subset C(x)$ for any $x \in \mathbb{R}^d$,

(here $d_{\mathcal{H}}$ denotes the Hausdorff distance). For $x, y \in \mathbb{R}^d$, let $\mathcal{F}_{x,y}$ be the set of all the trajectories $X(\cdot)$ defined by the differential inclusion

$$\dot{X}(t) \in C(X(t)),\ X(0) = x,\ X(T) = y,$$

for some $T = T(X(\cdot)) > 0$. Note that, because of the assumptions on the map $C(x)$, $\mathcal{F}_{x,y}$ is not empty. The function $d_C : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, defined by

$$d_C(x, y) = \inf_{\mathcal{F}_{x,y}} T(X(\cdot)), \tag{15}$$

is a distance function, equivalent to the Euclidean distance.

Define a Hamiltonian $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ as the support function of the convex set C, i.e.

$$H(x,p) = \sup_{q \in C(x)} p \cdot q. \tag{16}$$

Then, $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a continuous function and satisfies the following properties

$$\begin{gathered} H(x,0) = 0, \; H(x,p) \geq 0; \\ H(x,p) \text{ is convex and positive homogeneous in } p, \\ \text{i.e. for } \lambda > 0, \; H(x, \lambda p) = \lambda H(x,p); \\ |H(x,p) - H(x,q)| \leq L|x-y|(1+|p|). \end{gathered}$$

Moreover, for any $y \in \mathbb{R}^d$, the function $u : \mathbb{R}^d \to \mathbb{R}$, defined by $u(x) = d_C(y,x)$, is the unique viscosity solution of the problem

$$\begin{cases} H(x, Du) = 1, & x \in \mathbb{R}^d, \\ u(y) = 0. \end{cases} \tag{17}$$

Remark

Some examples of distance defined by a convex map C are

1. *if* $C(x) = \{p \in \mathbb{R}^d : \|p\|_s = (\sum_{i=1}^{d} |p_i|^s)^{1/s} \leq 1\}$ *for* $s > 1$, *then* d_C *is the Minkowski distance* $d_C(x, y) = \|x - y\|_s$ *and* $H(x, p) = |p|^2 / \|p\|_s$;
2. *if* $C(x) = a(x)B(0, 1)$, *where* $a(x) \geq \delta > 0$, *then* $H(x, p) = a(x)|p|$;
3. *if* $C(x) = A(x)^{\frac{1}{2}} B(0, 1)$, *where* A *is a positive definite matrix such that* $A(x)\xi \cdot \xi \geq \delta > 0$ *for* $\xi \in \mathbb{R}^d$, *then* d_C *is the Riemannian distance induced by the matrix* A *on* $\mathbb{R}^d$ *and* $H(x, p) = \sqrt{A(x)p \cdot p}$.

Given a set of generators $\{y_k\}_{k=1}^K$, $y_k \in \overline{\Omega}$, we define a geodesic Voronoi tessellation of Ω as the union of the geodesic Voronoi diagrams

$$V(y_k) = \{x \in \Omega : \, d_C(x, y_k) = \min_{j=1,\dots,K} d_C(x, y_j)\} \tag{18}$$

(the point of $V(y_k) \cap V(y_j)$ are assigned to the diagram with the smaller index).

Definition

A geodesic Voronoi tessellation $\{V(y_k)\}_{k=1}^K$ of Ω is said to be a geodesic centroidal Voronoi tessellation (GCVT in short) if, for each $k = 1, \dots, K$, the generator y_k of $V(y_k)$ coincides with the centroid of $V(y_k)$, i.e.

$$\int_{V(y_k)} \rho(x) d_C(y_k, x) dx = \min_{z \in V(y_k)} \int_{V(y_k)} \rho(x) d_C(z, x) dx. \tag{19}$$

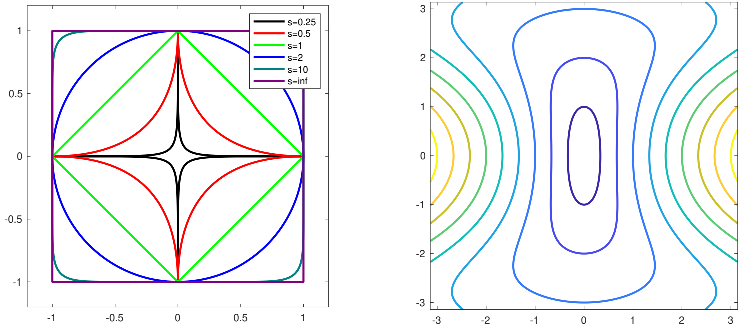


Figure: Unitary balls for the Minkowski distance for various values of s (left) and a Riemann distance induced by $A(x, y) = ((R + r\cos y)^2, 0; 0, r^2)$ for $R = 1$, $r = 0.5$, corresponding to parametrization of an unitary torus in $\mathbb{R}^3$.

Consider the functional with $V(y_k)$ as before

$$\mathcal{I}_{d_C}(y_1,\dots,y_k)=\sum_{k=1}^{K}\int_{V(y_k)} d_C(y_k,x)^2\rho(x)dx, \tag{20}$$

It is possible to prove that the critical points of the functional determine GCVTs of the domain Ω and the corresponding Lloyd algorithm converges to a (local) minimum of $\mathcal{I}_{d_C}$.
We characterize GCVTs of Ω via the following system of HJ equations

$$\begin{cases} H(x,Du_k)=1, \qquad x\in\Omega,\\ u_k(\mu_k)=0,\\ S_u^k=\{x\in\mathbb{R}^d:\ u_k(x)=\min_{j=1,\dots,K}u_j(x)\},\\ \int_{S_u^k}\rho(x)u_k(x)dx=\min\{\int_{S_u^k}\rho(x)u_y(x)dx : u_y \text{ solution of (17) with } y\in S_u^k\}\end{cases} \tag{21}$$

for $k=1,\dots,K$.

Proposition

The following conditions are equivalent:

(i) *Let $(y_1,\dots,y_K)$ be a critical point of the functional $\mathcal{I}_{d_C}$ with geodesic Voronoi diagrams $V(y_k)$. Then, there exists a solution of (21) such that $\mu_k=y_k$ and $S_u^k=V(y_k)$.*

(ii) *Given a solution $u=(u_1,\dots,u_K)$ of (21), then $(\mu_1,\dots,\mu_K)$ is a critical point of $\mathcal{I}_{d_C}$ with geodesic Voronoi diagrams $V(y_k)=S_u^k$.*

We observe that, in terms of (21), the Lloyd algorithm can be rewritten as follows: given an initial guess $(\mu^{(0),1}, \ldots, \mu^{(0),k})$, at $(n)^{th}$-step,

- Solve the K (uncoupled) HJ equations

$$\begin{cases} H(x, Du_k^{(n)}) = 1, \\ u_k^{(n)}(\mu^{(n),k}) = 0, \end{cases} \tag{22}$$

for $k = 1, \ldots, K$ and compute the Voronoi diagrams

$$S_u^{k,(n)} = \{x \in \Omega : \ u_k^{(n)}(x) = \min_{j=1,\ldots,K} u_j^{(n)}(x)\}, \quad k = 1, \ldots, K.$$

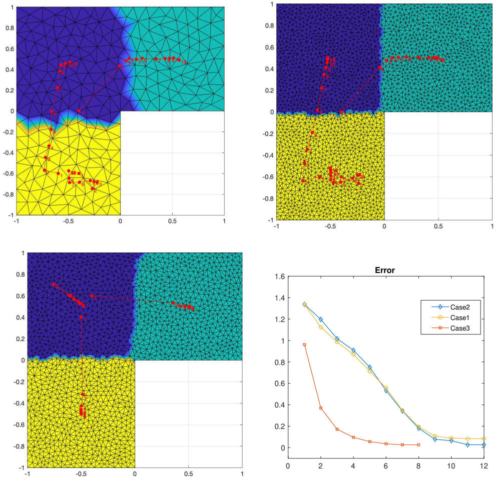
- Compute the new centroids $\mu^{(n+1),k}$ via the optimization problem

$$\int_{S_u^{k,(n)}} \rho(x) u_{\mu^{(n+1),k}}(x) dx = \min \Big\{ \int_{S_u^{k,(n)}} \rho(x) u_y(x) dx : \\ u_y \text{ solution of (17) with } y \in S_u^{k,(n)} \Big\}. \tag{23}$$

In the first step of the iterative procedure, it is sufficient to solve problem (22) the set Ω, the support of the density ρ.

Test 3. A verification test.

In this case, the Chebyshev distance (i.e. $s \to \infty$) has an easly guessed optimal tessellation.



Test 4. Riemannian manifolds

$$A_{cyl}(x,y) = \begin{pmatrix} r^2 & 0 \\ 0 & 1 \end{pmatrix}, \; A_{torus} = \begin{pmatrix} (R + r\cos y)^2 & 0 \\ 0 & r^2 \end{pmatrix}, \; A_{hyp} = \begin{pmatrix} 1+y^2 & xy \\ xy & 1+x^2 \end{pmatrix}.$$

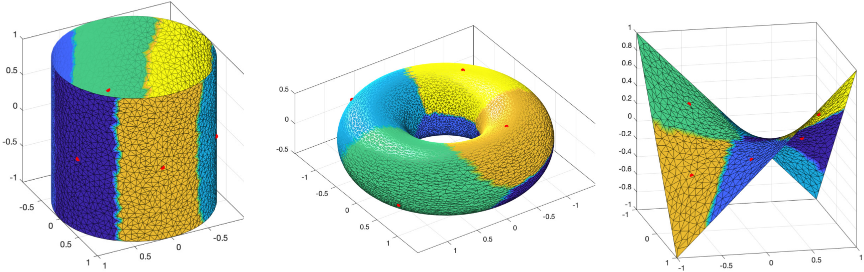


Figure: Three tessellations on two-dimensional manifolds. Respectively, a cylinder, a torus, a hyperbolic paraboloid. The parameters are set $K = 6$, $\Delta x = 0.01, 0.004, 0.004$. The position of the centroids in marked with red dots.

A system of HJ equations for centroidal power diagrams

We consider a generalization of centroidal Voronoi diagrams, called centroidal power diagrams.

Given a set of K distinct points $\{y_i\}_{i=1}^K$ in Ω and K real numbers $\{w_i\}_{i=1}^K$, the power diagrams generated by the couples (y_i, w_i) are defined by

$$V(y_i, w_i) = \{x \in \Omega : |x - y_i|^2 - w_i = \min_{j=1,\dots,K} (|x - y_j|^2 - w_j)\}. \quad (24)$$

As Voronoi diagrams, power diagrams provide a tessellation of the domain Ω, i.e. $V(y_i, w_i) \cap V(y_j, w_j) = \emptyset$ for $i \neq j$ and $\cup_{i=1}^K V(y_i, w_i) = \overline{\Omega}$.

- whereas Voronoi diagrams are always non empty, some of the power diagrams may be empty
- Power diagrams reduce to Voronoi diagrams if the weights w_i coincide
- the weights vector $w = (w_1, \dots, w_k)$ allows to impose additional constraints on the resulting tessellation.

Long story short, we propose the following HJ system for the characterization of the solutions

$$\begin{cases} |Du_k| = 2|x-\mu_k|^2, & x \in \Omega, \\ u_k(\mu_k) = -\omega_k, \\ S_u^k = \{x \in \mathbb{R}^d : \ u_k(x) = \min_{j=1,\dots,K} u_j(x)\} \\ \mu_k = \frac{\int_{S_u^k} x\rho(x)dx}{\int_{S_u^k} \rho(x)dx}, \\ \pi(S_u^k) = c_k. \end{cases} \tag{25}$$

The system (25) depends on the $2K$ parameters (μ_k, ω_k). If there exists a solution $u = (u_1, \dots, u_k)$ to the previous system, then $u_k = -\omega_k + |x-\mu_k|^2$, μ_k is the centroid of S_u^k. Moreover

$$S_u^k = \left\{ x \in \mathbb{R}^d : -w_k + |x-y_k|^2 = \min_{j=1,\dots,K} \{-w_j + |x-y_j|^2\} \right\} = V(y_k, w_k),$$

where $V(y_k, w_k)$ is defined as in (24), and $\pi(S_u^k) = c_k$. Hence $\{S_u^k\}_{k=1}^K$ gives a centroidal power diagram of Ω realizing the capacity constraint.

A PDE algorithm for centroidal power diagrams

Initialize $(\mu^{(0)}, w^{(0)}) = (\mu^{(0),1}, \ldots, \mu^{(0),K}, w^{(0),1}, \ldots, w^{(0),K})$ (centroids and weights). Iterate

(i) For $k = 1, \ldots, K$ and $j_k = \mathrm{argmin}_{i=1,\ldots,N}|X_i - \mu^{(n),k}|$, solve the problem

$$\begin{cases} G_i(U^{(n),k}) = 2|X_k - \mu^{(n),k}|, \quad i = 1, \ldots, N, \\ U^{(n),k}_{j_k} = -w^{(n-1)}_k, \end{cases} \tag{26}$$

and define $\mathcal{S}^{(n+1),k} = \bigcup \left\{ T_i : \ i \text{ is s.t. } U_i^{(n),k} = \min_{j=1,\ldots,K} U_i^{(n),j} \right\}$.

(ii) Compute the new centroids points

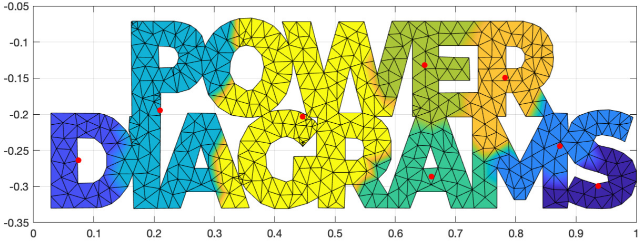
$$\mu^{(n+1),k} = \frac{\sum_{T_i \in \mathcal{S}^{(n+1),k}} X_i |T_i| \rho(X_i)}{\sum_{T_i \in \mathcal{S}^{(n+1),k}} |T_i| \rho(X_i)}. \tag{27}$$

(iii) Compute the new weights $w^{(n+1),k}$ as local maximum of the Lagrangian function

$$L(Y, w) = \sum_{i=1}^{k} \sum_{X_j \in \mathcal{S}^{(n+1),k}} \rho(X_j) d_C^2(Y, X_j) - \sum_{i=1}^{k} w_k(\pi(\mathcal{S}^{(n+1),k}) - c_k)$$

till meeting a stopping criterion as

$$\max\{|\mu^{(n+1),k} - \mu^{(n),k}|, |\omega^{(n+1),k} - \omega^{(n),k}|\} < \varepsilon.$$



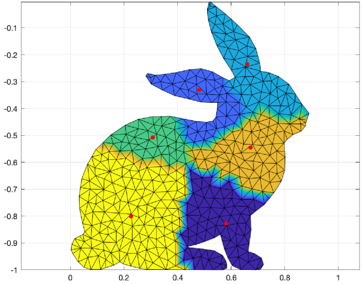


Figure: The parameters are set $K = 8$, $c = (0.33, 0.22, 0.1, 0.1, 0.1, 0.05, 0.05, 0.05)$, $\Delta x = 0.002$ (above) $K = 6$, $c = (0.25, 0.15, 0.15, 0.15, 0.15, 0.10)$, $\Delta x = 0.002$ (below).

Conclusions

- PDE theory is a robust framework to solve classic (and less traditional) tessellation problems. The main advantage of this approach is the high adaptability of the framework to specific variations of the problem (presence of constraints, non-conventional distance functions, etc.).
- This increased adaptability comes with a precise cost. A PDE approach is more computationally demanding than other methods available in the literature.
- The recent developments of numerical methods for nonlinear PDEs, and the increment of the accessibility to more powerful computational resources at any level, make these techniques progressively more appealing in many applicative contests.

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