Over-relaxation Lloyd Method for Computing Centroidal Voronoi Tessellations

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- Given an open convex set $\Omega \subseteq \mathbb{R}^N$, a set of subregions $\{V_i\}_{i=1}^n$ is called a *tessellation* of Ω if $V_i \cap V_j = \emptyset$ for $i \neq j$ and $\cup_{i=1}^n \bar{V}_i = \bar{\Omega}$.

- Let $\|\cdot\|$ denote denote the Euclidean distance. Given a set of points $\{\mathbf{z}_i\}_{i=1}^n$ in Ω, the *Voronoi region* V_i corresponding to the point $\mathbf{z}_i$ is defined by:

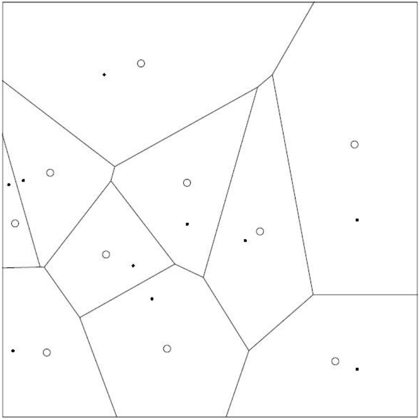
$$V_i = \{\mathbf{x} \in \Omega : \|\mathbf{x} - \mathbf{z}_i\| < \|\mathbf{x} - \mathbf{z}_j\| \ \text{ for } \ j = 1, \ldots, n, \ j \neq i\} \tag{1.1}$$

The set $\{V_i\}_{i=1}^n$ is called a *Voronoi tessellation* or *Voronoi diagram* of Ω; $\{\mathbf{z}_i\}_{i=1}^n$ is referred to as the *generating points* or *generators*.

- Given a density function ρ defined on Ω, the *mass centroid* of a subregion V of Ω is defined by

$$\mathbf{z}^* = \frac{\int_V \mathbf{x}\rho(\mathbf{x})\,\mathrm{d}\mathbf{x}}{\int_V \rho(\mathbf{x})\,\mathrm{d}\mathbf{x}} \tag{1.2}$$

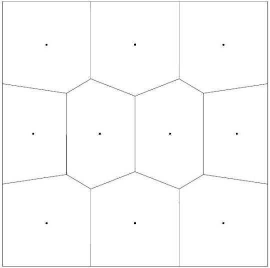
In general, arbitrarily chosen generators are not the mass centroids of their associated Voronoi regions.



- If the generators coincide with the mass centroids of their corresponding Voronoi regions, i.e.

$$\mathbf{z}_i = \mathbf{z}_i^*, \quad i = 1, \ldots, n,$$

then we call the tessellation $\{V_i\}_{i=1}^n$ defined by (1) a *Centroidal Voronoi Tessellation* (CVT) of Ω.



- Given a set of points $\{\mathbf{z}_i\}_{i=1}^n$ and a tessellation of Ω $\{V_i\}_{i=1}^n$, we may define a *energy functional* for the pair $(\{\mathbf{z}_i\}_{i=1}^n, \{V_i\}_{i=1}^n)$ by:

$$\mathcal{K}(\{\mathbf{z}_i\}_{i=1}^n, \{V_i\}_{i=1}^n) = \sum_{i=1}^n \int_{V_i} \rho(\mathbf{x}) \|\mathbf{x} - \mathbf{z}_i\|^2 \, \mathrm{d}\mathbf{x} \qquad (1.3)$$

- Du, Faber, Gunzburger (1996) showed that, a necessary condition for $\mathcal{K}$ to be minimized is that $V_i's$ are the Voronoi regions corresponding to $\mathbf{z}_i's$ and, simultaneously, the $\mathbf{z}_i's$ are the centroids of the corresponding $V_i's$, that is, $\{\mathbf{z}_i, V_i\}_{i=1}^n$ is a CVT of Ω.

Applications:

- image processing and analysis
- vector quantization and data analysis
- resource optimization
- optimal placement of sensors and actuators for control
- cell biology and territorial behavior of animals
- model reduction
- point sampling
- meshless computing
- mesh generation and optimization
- numerical PDEs
- geophysical flows
- computer graphics mobile sensing networks

CVT Construction Problem

Given

a region $\Omega \subseteq \mathbb{R}^N$

a positive integer n

a density function $\rho(x)$ defined for $x \in \Omega$

find

a n-point CVT of Ω with respect to the given density function ρ

Algorithm 1. (**Lloyd method**).
Given a set Ω, a density function $\rho(x)$ defined on $\bar{\Omega}$, and a positive integer n.

1. Choose an initial set of n points $\{\mathbf{z}_i\}_{i=1}^n$ in Ω, e.g., by using a Monte Carlo method.
2. Construct the corresponding Voronoi tessellations $\{V_i\}_{i=1}^n$.
3. Compute the mass centroids of these Voronoi regions. Let these be the new $\{\mathbf{z}_i\}_{i=1}^n$.
4. Repeat until we meet some convergence criterion.

Algorithm 2. (**Over-relaxation Lloyd method**).
Given a set Ω, a density function $\rho(x)$ defined on $\bar{\Omega}$, and a positive integer n.

1. Choose an initial set of n points $\{\mathbf{z}_i\}_{i=1}^n$ in Ω, e.g., by using a Monte Carlo method.
2. Construct the corresponding Voronoi tessellations $\{V_i\}_{i=1}^n$.
3. Compute the mass centroids $\{\mathbf{z}_i^*\}_{i=1}^n$ of these Voronoi regions Update $\{\mathbf{z}_i\}_{i=1}^n$ using $\mathbf{z}_i = \omega \mathbf{z}_i^* + (1-\omega)\mathbf{z}_i, \qquad i = 1, \ldots, n$ where $0 < \omega \leq 2$.
4. Repeat until we meet some convergence criterion.

Let the mappings $T_i : \mathbb{R}^{nN} \to \mathbb{R}^N$, $i = 1, \ldots, n$ be defined by:

$$T_i(\mathbf{Z}) = \frac{\int_{V_i(\mathbf{Z})} \mathbf{x}\rho(\mathbf{x})\,\mathrm{d}\mathbf{x}}{\int_{V_i(\mathbf{Z})} \rho(\mathbf{x})\,\mathrm{d}\mathbf{x}}$$

where $\mathbf{Z} = (\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_n)^T$ and $V_i(\mathbf{Z})$ denotes the Voronoi region associated with $\mathbf{z}_i$ generated by $\mathbf{Z}$. Then define the Lloyd map $\mathbf{T}$ to be

$$\mathbf{T} = (T_1, T_2, \ldots, T_n)^T.$$

Lloyd method is just the iterative process:

$$\mathbf{Z}^{(n+1)} = \mathbf{T}(\mathbf{Z}^{(n)}), \qquad n = 0, 1, \ldots.$$

Centroidal Voronoi tessellations are fixed points of $\mathbf{T}$.

We claim that when $\mathbf{Z}^{(n)}$ is close to a CVT generator $\mathbf{Z}^*$, one can approximate the Lloyd map by,

$$\mathbf{T}(\mathbf{Z}^{(n)}) \approx \widetilde{\mathbf{T}}\mathbf{Z}^{(n)} + \mathbf{b} \tag{4.1}$$

where $\widetilde{\mathbf{T}}$ represents the Jacobian matrix of $\mathbf{T}$ at $\mathbf{Z}^*$ and $\mathbf{b}$ is some vector which is determined by the set Ω.

Proof: Let $\mathbf{Z}^*$ be the fixed point of T, i.e, $\mathbf{T}(\mathbf{Z}^*) = \mathbf{Z}^*$.
Since $\mathbf{T}$ is the Lloyd's map,

$$\mathbf{Z}^{(n+1)} = \mathbf{T}(\mathbf{Z}^{(n)})$$
$$\mathbf{T}(\mathbf{Z}^{(n)}) - \mathbf{T}(\mathbf{Z}^*) = \mathbf{Z}^{(n+1)} - \mathbf{Z}^*$$
$$\widetilde{\mathbf{T}} \cdot (\mathbf{Z}^{(n)} - \mathbf{Z}^*) \approx \mathbf{Z}^{(n+1)} - \mathbf{Z}^*$$
$$\mathbf{T}(\mathbf{Z}^{(n)}) = \mathbf{Z}^{(n+1)} \approx \mathbf{Z}^* + \widetilde{\mathbf{T}}(\mathbf{Z}^{(n)} - \mathbf{Z}^*)$$
$$\mathbf{T}(\mathbf{Z}^{(n)}) = \mathbf{Z}^{(n+1)} \approx \widetilde{\mathbf{T}} \cdot \mathbf{Z}^{(n)} + (\mathbf{Z}^* - \widetilde{\mathbf{T}} \cdot \mathbf{Z}^*)$$

So we have $\mathbf{T}(\mathbf{Z}^{(n)}) \approx \widetilde{\mathbf{T}}\mathbf{Z}^{(n)} + \mathbf{b}$, where $\mathbf{b} = \mathbf{Z}^* - \widetilde{\mathbf{T}} \cdot \mathbf{Z}^*$.

Apply the over-relaxation scheme in the Lloyd iteration, we have

$$\begin{aligned}\mathbf{Z}^{(n+1)} &= \omega\mathbf{T}(\mathbf{Z}^n) + (1-\omega)\mathbf{Z}^n \\ &\approx [\omega\widetilde{\mathbf{T}} + (1-\omega)\mathbf{I}]\mathbf{Z}^n + \omega\mathbf{b}\end{aligned} \tag{4.2}$$

Let $\vec{\mathbf{e}}^{\,n} = \mathbf{Z}^n - \mathbf{Z}^*$ represent the error. Then from (4.2), we have $\vec{\mathbf{e}}^{\,n+1} = (\omega\widetilde{\mathbf{T}} + (1-\omega)\mathbf{I})\vec{\mathbf{e}}^{\,n}$ and thus

$$\|\vec{\mathbf{e}}^{\,n+1}\| \leq \|\omega\widetilde{\mathbf{T}} + (1-\omega)\mathbf{I}\| \cdot \|\vec{\mathbf{e}}^{\,n}\|.$$

The eigenvalues of $\omega\widetilde{\mathbf{T}} + (1-\omega)\mathbf{I}$ are $1-\omega(1-\rho_i)$ where ρ_i's are the eigenvalues of $\widetilde{\mathbf{T}}$. Let ρ_{max} and ρ_{min} denote the maximal and minimal eigenvalue of $\widetilde{\mathbf{T}}$ respectively.

One can show that $\max_i(|1-\omega(1-\rho_i)|)$ is minimized when

$$1-\omega(1-\rho_{max}) = -1+\omega(1-\rho_{min}).$$

Then we find the optimal parameter

$$\omega = \frac{2}{2-\rho_{max}-\rho_{min}} \tag{4.3}$$

One dimensional cases:
The Jacobian matrix at the fixed point $\mathbf{Z} = \mathbf{T}(\mathbf{Z})$ is a tridiagonal matrix with

$$\frac{\partial T_i}{\partial z_{i-1}} = \frac{(z_i - z_{i-1})}{4M_i}\rho(\frac{z_i + z_{i-1}}{2}),$$

$$\frac{\partial T_i}{\partial z_{i+1}} = \frac{(z_{i+1} - z_i)}{4M_i}\rho(\frac{z_i + z_{i-1}}{2}),$$

$$\frac{\partial T_i}{\partial z_i} = \frac{\partial T_i}{\partial z_{i-1}} + \frac{\partial T_i}{\partial z_{i+1}}$$

where $T_i(\mathbf{Z}) = \frac{1}{M_i}\int_{V_i} x\rho(x)\,\mathrm{d}x$, $M_i = \int_{V_i}\rho(x)\,\mathrm{d}x$.

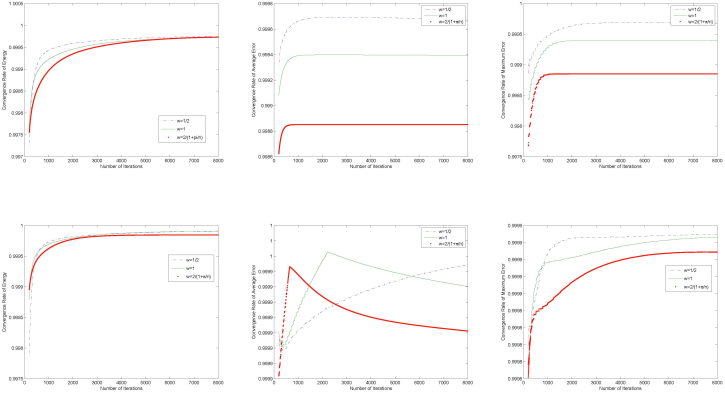
Particularly, for constant density, we have:

$$\mathbf{T} = \begin{pmatrix} 1/4 & 1/4 & 0 & \cdots & 0 & 0 & 0 \\ 1/4 & 1/2 & 1/4 & \cdots & 0 & 0 & 0 \\ 0 & 1/4 & 1/2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1/2 & 1/4 & 0 \\ 0 & 0 & 0 & \cdots & 1/4 & 1/2 & 1/4 \\ 0 & 0 & 0 & \cdots & 0 & 1/4 & 1/4 \end{pmatrix}$$

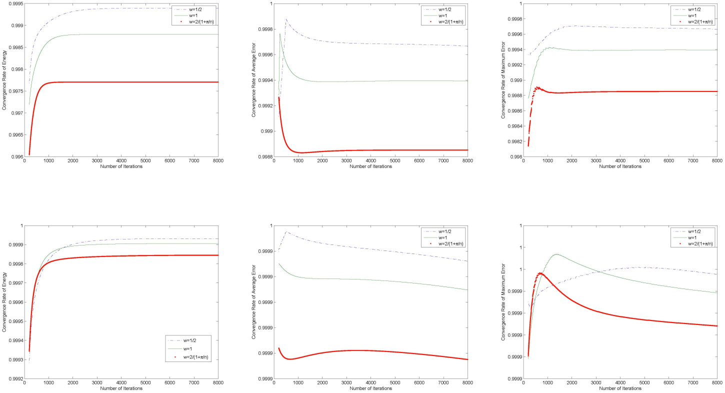
$$\rho_{max} \approx \cos^2\left(\frac{\pi}{2(n+1)}\right), \quad \rho_{min} = 0.$$

$$\omega \approx 2$$

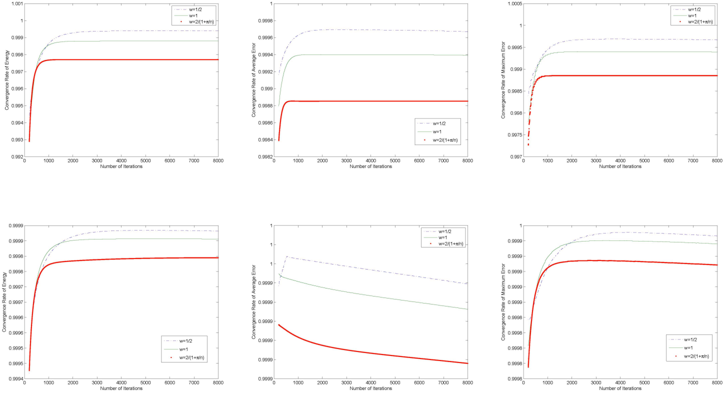
- In general, the over-relaxation parameter ω needs to lie between 0 and 2 to guarantee the method convergence.
- Analytically, we can approximate $\widetilde{\mathbf{T}}$ by the Jacobian matrix of $\mathbf{T}$ at $\mathbf{Z}^{(n)}$ when $\mathbf{Z}^{(n)}$ is close to the fixed point and then calculate an optimal over-relaxation parameter, but practically it is too costly. Actually we think any ω slightly smaller than 2 will be a good choice.
- We compare performance of the over-relaxation Lloyd method for some density functions in one ($\Omega = [0,1]$) and two dimensions ($\Omega = [0,1] \times [0,1]$) with three different over-relaxation parameters $\omega = 1, \frac{1}{2}, \frac{2}{1+\frac{\pi}{n}}$.
- The results show that the method with $\frac{2}{1+\frac{\pi}{n}}$ always perform the best.



1D example with $\rho(x) = 1$. Top: $n = 64$; bottom: $n = 256$.



1D example with $\rho(x) = e^{-2x}$. Top: $n = 64$; bottom: $n = 256$.



1D example with $\rho(x) = e^{-2x^2}$. Top: $n = 64$; bottom: $n = 256$.

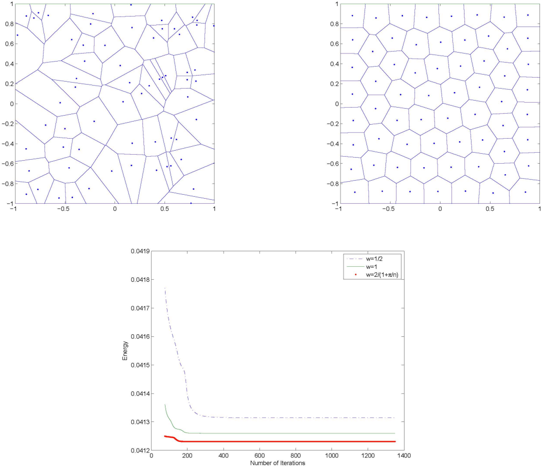


Figure 4. 2D example with $\rho(x) = 1$ and $n = 64$.

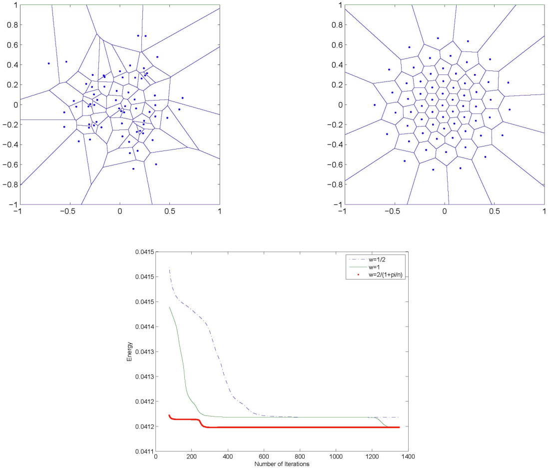


Figure 5. 2D example with $\rho(x) = 4e^{-8(x^2+y^2)}$ and $n = 64$.