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CONVERGENCE OF THE LLOYD ALGORITHM FOR COMPUTING CENTROIDAL VORONOI TESSELLATIONS*

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Abstract. Centroidal Voronoi tessellations (CVTs) are Voronoi tessellations of a bounded geometric domain such that the generating points of the tessellations are also the centroids (mass centers) of the corresponding Voronoi regions with respect to a given density function. Centroidal Voronoi tessellations may also be defined in more abstract and more general settings. Due to the natural optimization properties enjoyed by CVTs, they have many applications in diverse fields. The Lloyd algorithm is one of the most popular iterative schemes for computing the CVTs but its theoretical analysis is far from complete. In this paper, some new analytical results on the local and global convergence of the Lloyd algorithm are presented. These results are derived through careful utilization of the optimization properties shared by CVTs. Numerical experiments are also provided to substantiate the theoretical analysis.

Key words. centroidal Voronoi tessellations, k-means, optimal vector quantizer, Lloyd algorithm, global convergence, convergence rate

AMS subject classifications. 65D99, 65C20

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1. Introduction.

A centroidal Voronoi tessellation (CVT) is a special Voronoi tessellation of a given set such that the associated generating points are the centroids (centers of mass) of the corresponding Voronoi regions with respect to a predefined density function [7]. CVTs are indeed special as they enjoy very natural optimization properties which make them very popular in diverse scientific and engineering applications that include art design, astronomy, clustering, geometric modeling, image and data analysis, resource optimization, quadrature design, sensor networks, and numerical solution of partial differential equations [1, 2, 3, 4, 7, 8, 9, 10, 11, 13, 14, 17, 15, 26, 29, 30, 31, 39, 44, 45]. In particular, CVTs have been widely used in the design of optimal vector quantizers in electrical engineering [25, 28, 40, 43]. They are also related to the so-called method of k-means [27] in clustering analysis. CVTs can also be defined in more general cases such as those constrained to a manifold [12, 11] or those corresponding to anisotropic metrics [16, 18], and other abstract settings [7, 9].

For modern applications of the CVT concept in large-scale scientific and engineering problems, it is important to develop robust and efficient algorithms for constructing CVTs in various settings. Historically, a number of algorithms have been studied and widely used [7, 19, 25, 27, 38]. A seminal work is the algorithm first developed in the 1960s at Bell Laboratories by S. Lloyd which remains to this day one of the most popular methods due to its effectiveness and simplicity. The algorithm was later officially published in [35]. It is now commonly referred to as the Lloyd algorithm and is the main focus of this paper.

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The Lloyd algorithm has many elegant and simple interpretations [7], but to present it more rigorously, we begin with a more detailed description of the CVT. First of all, we recall the concept of the Voronoi tessellation (or Voronoi diagram). A Voronoi tessellation refers to a tessellation of a given domain $\Omega \in \mathbb{R}^N$ by the Voronoi regions $\{V_i\}_{i=1}^k$ associated with a set of given *generating points* or *generators* $\{\mathbf{z}_i\}_{i=1}^k \subset \Omega$ [22, 33, 41]. For each i, $\{V_i\}_{i=1}^k$ consists of all points in the domain Ω that are closer to $\mathbf{z}_i$ than to all the other generating points. For a given density function ρ defined on Ω, we may define the centroids, or mass centers, of regions $\{V_i\}_{i=1}^k$ by

$$\mathbf{z}_i^* = \frac{\displaystyle\int_{V_i} \mathbf{y}\rho(\mathbf{y})\, d\mathbf{y}}{\displaystyle\int_{V_i} \rho(\mathbf{y})\, d\mathbf{y}}\,. \tag{1.1}$$

Then, a CVT refers to a Voronoi tessellation for which the generators themselves are the centroids of their respective Voronoi regions, that is, $\mathbf{z}_i = \mathbf{z}_i^*$ for all i. We refer to [7] for a more comprehensive review of the mathematical theory and diverse applications of CVTs.

In the seminal work of Lloyd on the least square quantization [35], one of the algorithms proposed for computing the CVTs (referred to as the optimal quantizers in the particular setting) is an iterative algorithm consisting of the following simple steps: starting from an initial Voronoi tessellation corresponding to an old set of generators, a new set of generators is defined by the mass centers of the Voronoi regions. This process is continued until a certain stopping criterion is met. With the notation given above, the Lloyd algorithm for constructing CVTs can be described more precisely by the following procedure.

ALGORITHM 1.1 (Lloyd algorithm for computing CVTs).

Input:

Ω, the domain of interest; *ρ, a density function defined on Ω;*
k, number of generators; *$\{\mathbf{z}_i\}_{i=1}^k$, the initial set of generators.*

Output:

$\{V_i\}_{i=1}^k$, a CVT with k generators $\{\mathbf{z}_i\}_{i=1}^k$ in Ω.

Iteration:

1. *Construct the Voronoi tessellation $\{V_i\}_{i=1}^k$ of Ω with generators $\{\mathbf{z}_i\}_{i=1}^k$.*
2. *Take the mass centroids of $\{V_i\}_{i=1}^k$ as the new set of generators $\{\mathbf{z}_i\}_{i=1}^k$.*
3. *Repeat procedures* 1 *and* 2 *until some stopping criterion is met.*

Given a set of points $\{\mathbf{z}_i\}_{i=1}^k$ and a tessellation $\{V_i\}_{i=1}^k$ of the domain, we may define the *energy functional* or the *distortion value* for the pair $(\{\mathbf{z}_i\}_{i=1}^k, \{V_i\}_{i=1}^k)$ by

$$\mathcal{H}\Big(\{\mathbf{z}_i\}_{i=1}^k, \{V_i\}_{i=1}^k\Big) = \sum_{i=1}^k \int_{V_i} \rho(\mathbf{y})|\mathbf{y} - \mathbf{z}_i|^2\, d\mathbf{y}\,.$$

The minimizer of $\mathcal{H}$ necessarily forms a CVT which illustrates the optimization property of the CVT [7]. Meanwhile, it is easy to see that the Lloyd algorithm is an energy descent iteration, which gives strong indications of its practical convergence.

The Lloyd algorithm sparked enormous research efforts in later years and its variants have been proposed and studied in many contexts for different applications [25, 28, 40, 43, 35, 24, 23, 32, 34, 36]. A particular extension was made in [30] to combine the deterministic features of the Lloyd algorithm with some random sampling techniques. Despite its great success in applications and a large number of studies over the last few decades, only limited theoretical results on the Lloyd algorithm have been obtained [7] and many fundamental issues remain open concerning its convergence.

In this paper, we present a systematic study on both the local and the global convergence properties of the Lloyd algorithm. A number of new global convergence theorems are rigorously proved, including the global convergence of subsequences for any density functions, the global convergence of the whole sequence in one-dimensional space, and the global convergence under some nondegeneracy conditions. We also present some theoretical studies on the local convergence properties of the Lloyd algorithm including estimates on the convergence rates. Some numerical results are also presented to substantiate our theoretical investigation. Many of the techniques employed in this paper, in fact, work for more general settings. As an illustration, we analyze the application of the Lloyd algorithm to the construction of the constrained CVTs on a manifold and present some similar convergence theorems.

The rest of the paper is organized as follows. We present our main convergence theorems and some detailed discussions in section 2, followed by the extensions to more general settings that are considered in section 3 and numerical results that are given in section 4. Conclusions are drawn in section 5.

2. Convergence. Since Lloyd's pioneering work, many studies have been made on the convergence of the iteration [21, 24, 32, 36]. For example, the local convergence has been proved for strictly *logarithmically concave* density functions in the one-dimensional space [32]. An extension to CVTs defined on a circle is given in [12]. The convergence analysis in multidimensional space for general density functions is far from complete. There are very few known conditions that guarantee the global convergence. We now present some new results that have not been previously explored in the literature.

For clarity, since a Voronoi tessellation is defined using a point set with k points $\mathbf{Y} = \{\mathbf{y}_i\}_{i=1}^k$ as the respective generators, let us redefine the *energy functional*, or the *distortion value*, as a functional for a pair $(\mathbf{Y}, \mathbf{Z})$ with $\mathbf{Z} = (\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k) \in \mathbb{R}^{kN}$:

$$\mathcal{H}\Big(\mathbf{Y}, \mathbf{Z}\Big) = \sum_{i=1}^{k} \int_{V_i(\mathbf{Y})} \rho(\mathbf{y}) |\mathbf{y} - \mathbf{z}_i|^2 \, d\mathbf{y} \,,$$

where $\{V_i(\mathbf{Y})\}_{i=1}^k$ are the Voronoi regions with respect to $\{\mathbf{y}_i\}_{i=1}^k$. The Lloyd algorithm may be viewed as a fixed point iteration of the so-called Lloyd map [7], a mapping from a set of distinct generators $\{\mathbf{z}_i\}_{i=1}^k \subset \Omega \subset \mathbb{R}^N$ to the corresponding mass centers, defined by $\mathbf{T} = (\mathbf{T}_1, \mathbf{T}_2, \dots, \mathbf{T}_k)^T : \mathbb{R}^{kN} \to \mathbb{R}^{kN}$ with

$$\mathbf{T}_i(\mathbf{Z}) = \frac{\displaystyle\int_{V_i(\mathbf{Z})} \mathbf{y} \rho(\mathbf{y}) \, d\mathbf{y}}{\displaystyle\int_{V_i(\mathbf{Z})} \rho(\mathbf{y}) \, d\mathbf{y}} \,.$$

A set of generators of a centroidal Voronoi tessellation is obviously a fixed point of $\mathbf{T}$. Moreover, the Lloyd algorithm is equivalent to a fixed point iteration of $\mathbf{T}$:

$$\mathbf{Z}_n = \mathbf{T}(\mathbf{Z}_{n-1}) \qquad \text{for } n \geq 1 \,.$$

Notice that in general, the map $\mathbf{T}$ can be defined only on an open subset of $\Omega^k \subset \mathbb{R}^{kN}$ as we need to ensure that the denominators are nonzero, that is, the corresponding Voronoi regions are nonempty. This, in particular, implies that the generating points must be distinct. With this being noted, one needs to be cautious in applying general optimization theory concerning the convergence of energy descent algorithms [37] as such abstract theory often requires the compactness of the domain and the closedness of the associated map.

We now first quote some elementary facts for which one may find more detailed discussions in [7] and [41].

LEMMA 2.1. *Let ρ be a positive and smooth density function defined on a smooth bounded domain Ω. Then*

(1) *$\mathcal{H}$ is continuous and differentiable in $\bar{\Omega}^k \times \bar{\Omega}^k$;*

(2) $\mathcal{H}(\mathbf{Z}, \mathbf{T}(\mathbf{Z})) = \min_{\mathbf{Y}\in\bar{\Omega}^k} \mathcal{H}\Big(\mathbf{Z}, \mathbf{Y}\Big)$;

(3) $\mathcal{H}(\mathbf{Z}, \mathbf{Z}) = \min_{\mathbf{Y}\in\bar{\Omega}^k} \mathcal{H}(\mathbf{Y}, \mathbf{Z})$.

Next, we restate the strong connections between the map $\mathbf{T}$, the CVTs, and the Lloyd algorithm that we alluded to earlier.

LEMMA 2.2. *Let $\{\mathbf{Z}_n\}_1^\infty$ be the sequence of generating sets produced by the Lloyd algorithm. Then*

(1) $\mathbf{Z}_n = \mathbf{T}(\mathbf{Z}_{n-1})$;

(2) $\mathcal{H}(\mathbf{Z}_n, \mathbf{Z}_n) \leq \mathcal{H}(\mathbf{Z}_{n-1}, \mathbf{Z}_{n-1})$.

The first conclusion of the above lemma is obvious while the second one follows from properties (2) and (3) of Lemma 2.1 (for more details, see [7]). The results of Lemma 2.2 imply that the distortion (energy) values decrease when they are evaluated at consecutive iterations of the Lloyd algorithm; thus, the energy functional may be viewed as a descent function of the map $\mathbf{T}$, a fact that has been explored in [42], though the notion of a closed algorithm does not readily apply here due to the possible degeneracy of the Lloyd map $\mathbf{T}$ when some of the generating points either coincide or become arbitrarily close.

It is perhaps also interesting to note that the Lloyd algorithm may be viewed as an alternating variable algorithm for minimizing the energy functional, that is, in which one alternates between minimizing $\mathcal{H}(\mathbf{Y}, \mathbf{Z})$ with respect to $\mathbf{Y}$ and $\mathbf{Z}$. It is well known that there are examples of simple optimization problems with special objective functions for which such an alternating variable algorithm does not always converge. It is thus interesting to see whether the special features of the functional $\mathcal{H}$ can help us to establish the convergence of the Lloyd algorithm.

2.1. Existence of convergent subsequence. We now present some new convergence theorems concerning the Lloyd algorithm. It has been shown in [7] that if the density function is positive, except on a measure zero set, stationary points of the energy $\mathcal{H}$ are given by fixed points of the Lloyd map $\mathbf{T}$. The result below justifies that fixed points are attainable as a limit of Lloyd iterations.

THEOREM 2.3. *Any limit point $\mathbf{Z}$ of the Lloyd algorithm is a fixed point of the Lloyd map, and thus, $(\mathbf{Z}, \mathbf{Z})$ is a critical point of $\mathcal{H}$. Moreover, for an iteration started with a given initial guess, all elements in the set of its limit points share the same distortion value.*

Proof. The Lloyd algorithm produces a sequence $\{\mathbf{Z}_n\}$, which is bounded in $\bar{\Omega}^k$, and thus it has a convergent subsequence. Let $\mathbf{Z}$ be a limit point; then there exists a subsequence $\{\mathbf{Z}_{n_j}\}$ such that $\mathbf{Z}_{n_j} \to \mathbf{Z}$ as $n_j \to \infty$. Since the distortion values are monotonically decreasing, it follows that all limiting points must share the same distortion value.

Now, by properties of the iteration, $\mathcal{H}(\mathbf{Z}_n, \mathbf{Z}_n)$ is monotonically decreasing, so

$$\mathcal{H}\Big(\mathbf{Z}, \mathbf{Z}\Big) = \lim \mathcal{H}\Big(\mathbf{Z}_{n_j}, \mathbf{Z}_{n_j}\Big) = \inf \mathcal{H}\Big(\mathbf{Z}_n, \mathbf{Z}_n\Big)\ .$$

On the other hand, we know from Lemma 2.1 that

$$\mathcal{H}_1\Big(\mathbf{U},\mathbf{Z}_n\Big)\ |_{\mathbf{U}=\mathbf{Z}_n}=0\ .$$

Here we use the notation $\mathcal{H}_1$ to denote the partial derivatives with respect to all the components of the first argument (gradient with respect to the first argument $\mathbf{U}$) and $\mathcal{H}_2$ (the gradient) with respect to the second argument.

By continuity, we get

$$\mathcal{H}_1\Big(\mathbf{Z},\mathbf{Z}\Big)=0\ .$$

Now, if $\mathcal{H}_2(\mathbf{Z},\mathbf{U})\ |_{\mathbf{U}=\mathbf{Z}}=0$, $(\mathbf{Z},\mathbf{Z})$ is a critical point of $\mathcal{H}$ and we are done. Otherwise, there exists some $\mathbf{Y}$ such that

$$\mathcal{H}\Big(\mathbf{Z},\mathbf{Y}\Big)<\mathcal{H}\Big(\mathbf{Z},\mathbf{Z}\Big)\ .$$

Thus, for small enough δ, we have for large enough n_j that

$$\begin{aligned}\mathcal{H}\Big(\mathbf{Z}_{n_j},\mathbf{Y}\Big)&<\mathcal{H}\Big(\mathbf{Z},\mathbf{Y}\Big)+\delta\\&<\mathcal{H}\Big(\mathbf{Z},\mathbf{Z}\Big)\\&\le\mathcal{H}\Big(\mathbf{Z}_{n_j+1},\mathbf{Z}_{n_j+1}\Big)\\&\le\mathcal{H}\Big(\mathbf{Z}_{n_j},\mathbf{Z}_{n_j+1}\Big)\ .\end{aligned}$$

This contradicts the fact that

$$\mathcal{H}\Big(\mathbf{Z}_{n_j},\mathbf{Z}_{n_j+1}\Big)=\min_{\mathbf{Y}}\mathcal{H}\Big(\mathbf{Z}_{n_j},\mathbf{Y}\Big)\ .$$

Thus, the theorem is proved. ∎

The above theorem may be simply classified as a theorem for the global convergence of subsequences of the Lloyd algorithm. It leads to a more precise characterization of the algorithm and a hint on why it rarely fails, while also motivating the global convergence theorems for the whole sequence with some additional assumptions that we are going to present next.

2.2. Global convergence. As an immediate consequence of Theorem 2.3, we easily get the following result.

COROLLARY 2.4. *If the fixed point is unique, the Lloyd algorithm converges globally.*

The uniqueness of the fixed point has been established in some special cases in the literature. We will come back to this point later in the section. The uniqueness is obviously not a necessary condition, but we may in fact derive the following convergence theorem.

THEOREM 2.5. *If the set of fixed points with any particular distortion value is finite, the Lloyd algorithm converges globally.*

Proof. Convergence may fail only if the generated sequence possesses infinitely many jumps from a neighborhood of one fixed point to another. Suppose $\mathbf{U}$ and $\mathbf{V}$ are two fixed points with $||\mathbf{U}-\mathbf{V}||=\delta>0$. Denote the generated sequence of the Lloyd algorithm as $\mathbf{Z}_n$, i.e., $\mathbf{Z}_{n+1}=\mathbf{T}(\mathbf{Z}_n)$.

Suppose $\mathbf{Z}_{n_r} \to \mathbf{U}$ and $\mathbf{Z}_{n_l} \to \mathbf{V}$. Then for any $\delta > 0$, there exists $M > 0$ such that for all $n_r, n_l > M$ we have $||\mathbf{Z}_{n_r} - \mathbf{U}|| < \delta/3$ and $||\mathbf{Z}_{n_l} - \mathbf{V}|| < \delta/3$. The Lloyd map is continuous near the fixed points (see Proposition 3.5 in [7]), so M can be chosen to be suitably large to assure

$$||\mathbf{T}(\mathbf{Z}_{n_r}) - \mathbf{Z}_{n_r}|| < \delta/3.$$

Now suppose the sequence makes infinitely many jumps from subsequence $\{n_r\}$ to $\{n_l\}$; i.e., there are infinitely many μ, ν s.t. $n_{l_\mu} = n_{r_\nu} + 1$. Then $||\mathbf{T}(\mathbf{Z}_{n_{r_\nu}}) - \mathbf{V}|| = ||\mathbf{Z}_{n_{r_\nu}+1} - \mathbf{V}|| = ||\mathbf{Z}_{n_{l_\mu}} - \mathbf{V}||$. Hence

$$\delta = ||\mathbf{U} - \mathbf{V}|| \leq ||\mathbf{U} - \mathbf{Z}_{n_{r_\nu}}|| + ||\mathbf{Z}_{n_{r_\nu}} - \mathbf{T}(\mathbf{Z}_{n_{r_\nu}})|| + ||\mathbf{T}(\mathbf{Z}_{n_{r_\nu}}) - \mathbf{V}|| < \delta.$$

We get a contradiction. ∎

To this end, we have proved the global convergence of the Lloyd method in case the set of fixed points, Γ, does not have an accumulation point. Note that there are situations where Γ contains accumulation points and all points in Γ share the same distortion value. For example, consider the CVTs formed with two generators in a unit disc centered at the origin for the constant density function. Simple calculation shows that the critical points fill a circle of radius $4/(3\pi)$. That is, due to the rotation symmetry, any pair of points in the opposite ends of such a circle determines a CVT, and all the critical points share the same energy values. Of course, cases like this are very rare, so this fact does not present any difficulties for the convergence of the Lloyd algorithm in most practical applications.

We now present another result which further substantiates the global convergence of Lloyd algorithm in general.

THEOREM 2.6. *If the iterations in the Lloyd algorithm stay in a compact set, where the Lloyd map* $\mathbf{T}$ *is continuous, then the algorithm is globally convergent to a critical point of* $\mathcal{H}$.

Proof. The proposition follows from the global convergence theorem (GCT), [37] and similar arguments have been presented in [42]. Indeed, the Lloyd algorithm can be regarded as a descent method with the descent function given by $\mathcal{H}(\cdot, \mathbf{T}(\cdot))$. Let $\{\mathbf{Z}_n\}_{n=1}^{\infty}$ be a sequence generated by $\mathbf{Z}_{n+1} = \mathbf{T}(\mathbf{Z}_n)$. All $\mathbf{Z}_n$'s are contained in a compact set. If Γ is the set of solutions, $\mathcal{H}(\mathbf{Y}, \mathbf{T}(\mathbf{Y})) < \mathcal{H}(\mathbf{Z}, \mathbf{T}(\mathbf{Z}))$ for all $\mathbf{Z} \notin \Gamma$, $\mathbf{Y} \in \mathbf{T}(\mathbf{Z})$ and $\mathcal{H}(\mathbf{Y}, \mathbf{T}(\mathbf{Y})) = \mathcal{H}(\mathbf{Z}, \mathbf{T}(\mathbf{Z}))$ for all $\mathbf{Z} \in \Gamma$, $\mathbf{Y} \in \mathbf{T}(\mathbf{Z})$. The continuity implies the closedness of $\mathbf{T}$ in a compact set. Applying the GCT, we get the convergence of the sequence $\mathbf{Z}_n$, and the limit $\mathbf{Z}$ is a fixed point of $\mathbf{T}$; thus, the algorithm converges to a critical point of $\mathcal{H}$. ∎

We note that the compactness of the iteration seems to be intuitively true but it has not been rigorously justified in the literature. The difficulty is related to showing that during the iteration, the generators of the Voronoi regions do not get arbitrarily close as the Lloyd map is not well defined at degenerating points, where some of the generators may coincide.

2.3. The compactness in the one-dimensional case. Here, we take $\Omega = [a, b]$, a compact interval, let ρ be smooth and positive, and assume that $0 < M_1 \leq ||\rho||_{\infty,\Omega} \leq M_2 < \infty$. Let $M_c = M_2/M_1$; obviously, $M_c \geq 1$. We verify that throughout the Lloyd algorithm, the Voronoi regions remain nondegenerate (i.e., the generating points remain distinct); thus, it will lead to the global convergence.

First, we have the following simple fact.

LEMMA 2.7. *Given an interval $V = [z_l, z_r] \in \Omega$, let z^* be the mass centroid of V with respect to the density function ρ. Then we have*

$$L(V) \leq 2M_c \min(z^* - z_l,\ z_r - z^*), \tag{2.1}$$

where $L(V)$ denotes the length of V.

Proof. Without loss of generality, we suppose that $z^* - z_l \leq z_r - z^*$. By the definition of mass centroid, we have

$$z^* - z_l = \frac{\displaystyle\int_{z_l}^{z_r} (x - z_l)\rho(x)\, dx}{\displaystyle\int_{z_l}^{z_r} \rho(x)\, dx} \geq \frac{M_1}{2M_2}(z_r - z_l),$$

so we get

$$z_r - z_l \leq 2M_c(z^* - z_l).$$

With $z^* - z_l \leq z_r - z^*$, we get the inequality (2.1). ◻

Denote by $\{z_i^{(n)}\}_{i=1}^k$ $(z_1^{(0)} < z_2^{(0)} < \cdots < z_k^{(0)},\ n \geq 0)$ the positions of the generators after n iterations in the Lloyd method and by $\{V_i^{(n)} = (y_{i-1}^{(n)}, y_i^{(n)})\}_{i=1}^k$ the corresponding Voronoi regions. Clearly, $y_0^{(n)} = a$ and $y_k^{(n)} = b$. We now present a nondegeneracy result.

LEMMA 2.8. *For any $1 < i < k$, we have*

$$L(V_i^{(n+1)}) < \min\left(\frac{L(V_i^{(n)}) + L(V_{i+1}^{(n)})}{2} + L(V_{i-1}^{(n+1)}),\right.$$
$$\left.\frac{L(V_i^{(n)}) + L(V_{i-1}^{(n)})}{2} + L(V_{i+1}^{(n+1)})\right).$$

Proof. First we have

$$L(V_i^{(n+1)}) = \frac{z_{i+1}^{(n+1)} - z_i^{(n+1)}}{2} + \frac{z_i^{(n+1)} - z_{i-1}^{(n+1)}}{2}.$$

Since $z_i^{(n+1)} \in V_i^{(n)}$, $z_{i+1}^{(n+1)} \in V_{i+1}^{(n)}$, we know

$$\frac{z_{i+1}^{(n+1)} - z_i^{(n+1)}}{2} < \frac{L(V_i^{(n)}) + L(V_{i+1}^{(n)})}{2}.$$

With $L(V_{i-1}^{(n+1)}) > (z_i^{(n+1)} - z_{i-1}^{(n+1)})/2$, we get

$$L(V_i^{(n+1)}) < \frac{L(V_i^{(n)}) + L(V_{i+1}^{(n)})}{2} + L(V_{i-1}^{(n+1)}). \tag{2.2}$$

Similarly, we can prove that

$$L(V_i^{(n+1)}) < \frac{L(V_i^{(n)}) + L(V_{i-1}^{(n)})}{2} + L(V_{i+1}^{(n+1)}). \tag{2.3}$$

Combining (2.2) and (2.3), we complete the proof. ◻

This leads to the following uniform lower bound between the adjacent generators throughout the Lloyd algorithm.

PROPOSITION 2.9. *Let* $d_i^{(n)} = z_{i+1}^{(n)} - z_i^{(n)}$ *for* $i = 1, 2, \ldots, k-1$. *Then we have*

$$d_i^{(n)} > \frac{b-a}{k4^{2k-1}M_c^k}, \qquad n > k\,, \tag{2.4}$$

and consequently,

$$L(V_i^{(n)}) > \frac{b-a}{k4^{2k-1}M_c^k}, \quad 1 < i < k, \quad n > k\ , \tag{2.5}$$

and

$$L(V_i^{(n)}) > \frac{b-a}{2k4^{2k-1}M_c^k}, \quad i = 1 \text{ or } k, \quad n > k\ . \tag{2.6}$$

Proof. Let us consider any $d_i^{(n)}$ for $1 \le i \le k-1$ and $n > k$. Since $d_i^{(n)} = z_{i+1}^{(n)} - z_i^{(n)}$ and $y_i^{(n-1)} < z_{i+1}^{(n)}$, we have

$$y_i^{(n-1)} - z_i^{(n)} < d_i^{(n)}\ .$$

Then from Lemma 2.7, we have

$$L(V_i^{(n-1)}) < 2M_c d_i^{(n)}\ . \tag{2.7}$$

On the other hand, we know that $L(V_i^{(n-1)}) > (z_{i+1}^{(n-1)} - z_i^{(n-1)})/2$, which means

$$d_i^{(n-1)} < 2L(V_i^{(n-1)}) < 4M_c d_i^{(n)}\ .$$

Again by Lemma 2.7, we know that

$$L(V_{i-1}^{(n-2)}) < 8M_c^2 d_i^{(n)}\ .$$

Repeating this process, we have for $j = 1, \ldots, i$,

$$L(V_{i-j+1}^{(n-j)}) < 2^{2j-1} M_c^j d_i^{(n)}\ .$$

Now let us consider $j = i$. Clearly, $V_1^{(n-i)} = (a, y_1^{(n-i)})$, and we have

$$\begin{aligned} L(V_1^{(n-i+1)}) &< L(V_1^{(n-i)}) + L(V_2^{(n-i+1)}) \\ &< 2^{2i-1} M_c^i d_i^{(n)} + 2^{2i-3} M_c^{i-1} d_i^{(n)} \\ &< 4^i M_c^i d_i^{(n)}\ . \end{aligned}$$

Furthermore, by Lemma 2.8, we get

$$\begin{aligned} L(V_2^{(n-i+2)}) &< \frac{L(V_2^{(n-i+1)}) + L(V_1^{(n-i+1)})}{2} + L(V_3^{(n-i+2)}) \\ &< \frac{2^{2i-3} M_c^{i-1} d_i^{(n)} + 4^i M_c^i d_i^{(n)}}{2} + 2^{2i-5} M_c^{i-2} d_i^{(n)} \\ &< 4^i M_c^i d_i^{(n)}\ . \end{aligned}$$

Repeating this process, we have for $j = 1, \ldots, i-1$,

$$L(V_j^{(n-i+j)}) < 4^i M_c^i d_i^{(n)},$$

which means

$$L(V_{i-1}^{(n-1)}) < 4^i M_c^i d_i^{(n)} .$$

Using the same trick again and again, we finally arrive at

$$L(V_{i-j}^{(n-1)}) < 4^{i+j-1} M_c^i d_i^{(n)}, \qquad j = 1, \ldots, i-1.$$

Combining (2.7) and the above equation with $i, j \leq k$, we get

$$L(V_j^{(n-1)}) < 4^{2k-1} M_c^k d_i^{(n)}, \qquad j = 1, \ldots, i . \tag{2.8}$$

By symmetry, we also have

$$L(V_j^{(n-1)}) < 4^{2k-1} M_c^k d_i^{(n)}, \qquad j = i+1, \ldots, k .$$

Then, we get

$$b - a = L(\Omega) = \sum_{j=1}^{k} L(V_j^{(n-1)}) < k 4^{2k-1} M_c^k d_i^{(n)},$$

which implies (2.4), (2.5), and (2.6). ∎

We then have the following theorem.

THEOREM 2.10. *For any positive and smooth density function in one dimension and a given set of k distinct generators as a starting point, the Lloyd map is continuous at any of the iteration points.*

Proof. In order to show the continuity it is enough to justify the fact that Voronoi cells do not collapse. Indeed, after a sufficient number of steps, the latter is the direct consequence of Proposition 2.9. For the initial finite number of iterations, the continuity is obvious. ∎

Finally, using Theorems 2.6 and 2.10, we get Theorem 2.11.

THEOREM 2.11. *The Lloyd algorithm is globally convergent in one dimension for any positive and smooth density function.*

Proof. Using the result of Theorem 2.10, we see that we can define a compact set (away from the degenerating points) such that for any initial condition, the Lloyd iteration (the images of the Lloyd maps) will stay in such a compact set after sufficiently many steps. Thus, we may apply Theorem 2.6 to deduce the convergence of the algorithm. ∎

The above theorem provides an affirmative answer to the question of global convergence of the Lloyd algorithm for the one-dimensional interval case without any restrictive assumptions on the density functions. It remains an open problem to verify the same conclusion in the multidimensional case.

2.4. The logarithmic concave density for the one-dimensional case. Beyond the study on the global convergence, the characterization of the convergence rate is often also important in practice. For instance, one may inquire if a geometric convergence rate can be established. This is indeed verified in [7] for the constant density function corresponding to the unit interval $[0, 1]$, where, via the spectral analysis of $\mathbf{dT}$ at the minimizer, the established geometric convergence rate r is shown to satisfy

$$\sin^2\left(\frac{\pi}{2(k+1)}\right) \le r \le \sin^2\left(\frac{\pi}{2(k-1)}\right) , \tag{2.9}$$

so that asymptotically for large k (the total number of generators) the convergence rate is on the order of $1 - \pi^2/(4k^2)$, as verified by the numerical experiments in the next section.

In general, finding the convergence rate exactly is not possible, but estimates may be obtained from the analytical bounds of the $\|\mathbf{dT}\|$.

First, it follows from Theorem 2.10 that $\mathbf{T} : \Omega^k \to \Omega^k$ is a continuously differentiable mapping away from the degenerate points, where the generating points collapse. If this mapping $\mathbf{T}$ is a contraction, i.e., $||\mathbf{dT}|| < 1$ at all nondegenerate points, the contraction mapping theorem can be used to get a good estimate of the local convergence rate for the corresponding fixed point iteration, which in our case is the Lloyd algorithm. Moreover, the contraction mapping properties also imply that $\mathbf{T}$ has a unique fixed point $\mathbf{z}^*$ in the set of nondegenerate points upon a consistent ordering. Indeed, if there existed two fixed points $\mathbf{x} = \{x_i\}_{i=1}^k$ and $\mathbf{y} = \{y_i\}_{i=1}^k$, with components corresponding to generating points whose coordinates are ordered from small to large, that is, $x_i < x_{i+1}$ and $y_i < y_{i+1}$ for all indices i, then any point along the line segment $(1-t)\mathbf{x} + t\mathbf{y}$ would remain nondegenerate and thus, by uniform continuity, we may assume that

$$\sup_{0\le t\le 1} ||\mathbf{dT}(\mathbf{x} + t(\mathbf{y}-\mathbf{x}))|| \le \alpha(\mathbf{x},\mathbf{y}) < 1$$

for some constant $\alpha(\mathbf{x},\mathbf{y})$ independent of t. From the multidimensional form of the mean value theorem, we then get

$$||\mathbf{x}-\mathbf{y}|| = ||\mathbf{Tx}-\mathbf{Ty}|| \le \sup_{0\le t\le 1} ||\mathbf{dT}(\mathbf{x}+t(\mathbf{y}-\mathbf{x}))|| \, ||\mathbf{x}-\mathbf{y}|| \le \alpha ||\mathbf{x}-\mathbf{y}|| \,,$$

which is possible only if $\mathbf{x} = \mathbf{y}$; thus, we have the uniqueness. We refer to [32] for similar discussions.

The concept of logarithmic concavity has played an important role in the classification of one-dimensional density functions since it is a class of density functions for which the Lloyd maps can be shown to be contractions [7].

Let us take a closer look at the structure of the Jacobian $\mathbf{dT}$. By the notation of the previous section, for the one-dimensional case (i.e., $\Omega = [a, b]$), we have

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

$$\frac{\partial T_i}{\partial z_{i-1}} = \frac{\rho(z_i^-)(T_i - z_i^-)}{2R_i}, \qquad \text{and} \qquad \frac{\partial T_i}{\partial z_{i+1}} = \frac{\rho(z_i^+)(z_i^+ - T_i)}{2R_i}, \tag{2.10}$$

where $R_i = \int_{V_i} \rho(y)dy$ and $V_i = [z_i^-, z_i^+]$.

The following useful relation may be found in [7, 24]:

$$R_i^2\left(1 - \sum_j \frac{\partial T_i}{\partial z_j}\right) = \frac{1}{2}\int_{V_i}\int_{V_i} \rho(t)\rho(s)\left(\frac{\rho'(s)}{\rho(s)} - \frac{\rho'(t)}{\rho(t)}\right)(t-s)dt\ ds \tag{2.11}$$

at a fixed point $\mathbf{z} = \mathbf{T}(\mathbf{z})$.

Based on this, it can be shown that for the class of logarithmically concave functions (i.e., $(\log \rho)'' < 0$), the spectral radius of the Jacobi map is less than 1 in the neighborhood of a fixed point. In fact, it is easy to show that the same estimate holds for all points as the identity (2.11) remains universally true. Hence the fixed point of the Lloyd map is unique when the generators are ordered in an increasing manner. The following convergence of the Lloyd algorithm for the logarithmically concave case is easily one of the most popular results studied in the literature.

PROPOSITION 2.12. *In one dimension, in case of logarithmically concave density, the Lloyd algorithm converges globally to the unique fixed point.*

The class of logarithmically concave functions covers many densities used in practice, for instance, linear densities and normal distributions. Notice that the result quoted in Proposition 2.12 does not provide the estimate of the actual distance of the spectral radius from 1. We now focus on getting estimates on $\theta = 1 - ||\mathbf{dT}||$ more accurately. For this, we use a more precise measure of the logarithmic concavity for the density, that is, we assume that

$$\rho(t)\rho(s)\left(\frac{\rho'(s)}{\rho(s)} - \frac{\rho'(t)}{\rho(t)}\right)(t-s) \geq c_0^2(t-s)^2 \tag{2.12}$$

for some constant $c_0 > 0$ and any (t, s) except for a set of measure zero. Upon availability of an estimate of this type, the following conclusion can be reached:

$$1 - ||\mathbf{dT}|| \geq c_0^2 \min_i \left\{ R_i^{-2} \int_{V_i}\int_{V_i} (t-s)^2 dtds \right\} \sim \frac{c_0^2}{12} \min \left\{ \frac{h_i^2}{\rho(\zeta_i)^2} \right\}$$

for some $\zeta_i \in V_i$ and $h_i = z_i^+ - z_i^-$. Let $h = \min_i h_i$, the smallest Voronoi cell size, and $M = \sup_{x\in[0,1]} \rho(x)$; then we can rewrite the above result as follows.

LEMMA 2.13. *For any smooth density ρ satisfying* (2.12) *on the unit interval, the Lloyd algorithm is globally convergent with a geometric convergence rate no larger than*

$$||\mathbf{dT}|| \leq 1 - \frac{c_0^2}{12}\frac{h^2}{M^2} . \tag{2.13}$$

The convergence estimate obtained here essentially depends on characteristics c_0 and the relative size of a Voronoi cell in comparison with the density distribution. Since the minimizer of the energy gives a nondegenerate Voronoi diagram (Proposition 3.5 in [7]), there is a positive lower bound for the distance h in the neighborhood of the solution in terms of the density and the number of generators. Moreover, for large k, due to the asymptotic equipartition of energy property in one dimension [7], after sufficiently many iterations, one can roughly estimate each cell size as

$$h_i \sim k^{-1}\rho(\zeta_i)^{-1/3} \int_0^1 \rho^{1/3}(x)dx .$$

Thus, we have effectively $\theta = 1 - ||\mathbf{dT}|| \geq \left(\frac{c_1}{k}\right)^2$, where for large k,

$$c_1 \sim \frac{c_0}{\sqrt{12}M^{4/3}} \int_0^1 \rho^{1/3}(x)dx . \tag{2.14}$$

The estimate (2.14) in general tends to be rather pessimistic; for instance, for a linear perturbation of the constant density $\rho(x) = 1 - \epsilon x$ for a small ϵ, we have $c_1 \sim \frac{3}{4\sqrt{12}}(1-(1-\epsilon)^{4/3})$, which is significantly different from $\pi/2$ in the limit as $\epsilon \to 0$ (for the constant density case, c_1 can be estimated more accurately from the estimate (2.9) as $\pi/2$). This is due to the fact that the class of constant densities shares zero value of the parameter c_0. Nevertheless, it allows us to reach the conclusion that the geometric convergence rate for all densities satisfying (2.12) is comparable with that of the constant density in the sense that θ remains of the order k^{-2} for large values of k.

We expect that such a conclusion holds for even more general density functions, but the rigorous analysis is still not available.

3. Extensions to constrained CVTs. We now briefly illustrate how much of our earlier analysis can be extended to more general settings, where the concept of CVTs can be defined. The example to be used is of constrained CVTs on general surfaces as defined in [12].

Consider a compact and smooth surface $\mathbf{S} \subset \mathbb{R}^N$. Similar to the definition of conventional CVTs, for a given set of points $\{\mathbf{z}_i\}_{i=1}^k \in \mathbf{S}$, one may define their corresponding Voronoi regions on $\mathbf{S}$ by

$$V_i = \{\, \mathbf{x} \in \mathbf{S} \;:\; |\mathbf{x} - \mathbf{z}_i| < |\mathbf{x} - \mathbf{z}_j| \quad \text{for } j = 1, \dots, k,\, j \neq i \,\}. \tag{3.1}$$

For a density function ρ defined on the surface $\mathbf{S}$ and positive almost everywhere, one may encounter a problem with the original definition when one defines centroidal Voronoi tessellations $\{(\mathbf{z}_i, V_i)\}_{i=1}^k$ of $\mathbf{S}$: the mass centroids $\{\mathbf{z}_i^*\}_{i=1}^k$ of $\{V_i\}_{i=1}^k$ as defined by (1.1) do not in general belong to $\mathbf{S}$. For example, the mass centroid of any region on the surface of a sphere is always located in the interior of the sphere. Therefore, a generalized definition of a mass centroid on surfaces is needed. For each Voronoi region $V_i \subset \mathbf{S}$, we call $\mathbf{z}_i^c$ the *constrained mass centroid* of V_i on $\mathbf{S}$ if $\mathbf{z}_i^c$ is a solution of the following problem:

$$\min_{\mathbf{z} \in \mathbf{S}} F_i(\mathbf{z}), \qquad \text{where} \qquad F_i(\mathbf{z}) = \int_{V_i} \rho(\mathbf{x}) |\mathbf{x} - \mathbf{z}|^2 \, d\mathbf{x}\,. \tag{3.2}$$

The integral over $\{V_i\}$ is understood as a standard surface integration on $\mathbf{S}$. Note that the constrained mass centroid coincides with the conventional mass center if $\mathbf{S}$ is replaced by $\mathbb{R}^N$ and V_i is a convex subset of $\mathbb{R}^N$. Clearly, for each $i = 1, \dots, k$, $F_i(\cdot)$ is convex. Since $\mathbf{S}$ is compact and $\rho(\cdot)$ is continuous almost everywhere, there exists a constant C such that for any $\mathbf{z}_1, \mathbf{z}_2 \in \mathbf{S}$, we have

$$|F_i(\mathbf{z}_1) - F_i(\mathbf{z}_2)| = \left| \int_{V_i} \rho(\mathbf{x})(|\mathbf{x} - \mathbf{z}_1|^2 - |\mathbf{x} - \mathbf{z}_2|^2) \, d\mathbf{x} \right| \le C |\mathbf{z}_1 - \mathbf{z}_2|\,.$$

Thus, F_i is continuous and compact, and consequently we have the existence of solutions of (3.2), although the solution may not be unique.

We call the tessellation defined by (3.1) a *constrained centroidal Voronoi tessellation* (CCVT) if and only if the points $\{\mathbf{z}_i\}_{i=1}^k$ which serve as the generators associated with the Voronoi regions $\{V_i\}_{i=1}^k$ are the constrained mass centroids of those regions [12]. This definition of CCVT conforms with that of CVT for general spaces and clearly the energy $\mathcal{H}$ defined in (3.2) for CVTs is still valid for CCVTs. In Figure 1, we give two examples of CCVTs, one with six generators constrained to a circle

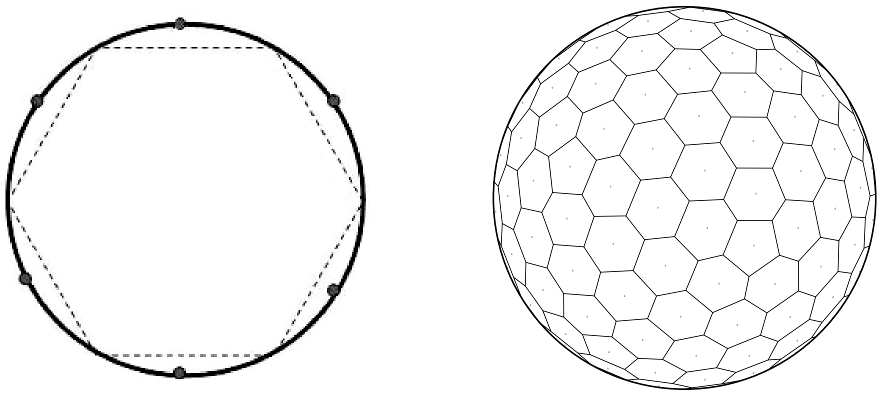

FIG. 1. *Examples of CCVTs for a circle (dots are for generators and dashes show the partition of the constrained Voronoi regions) and for a sphere (dots are generators and lines are planar projections of Voronoi edges). Only portion in one hemisphere is shown.*

(one-dimensional curve) and the other with 162 generators constrained to a sphere (two-dimensional surface). Both correspond to the constant density.

The following generalized Lloyd algorithm for computing CCVTs was proposed in [12].

ALGORITHM 3.1 (Lloyd algorithm for computing CCVTs).

Input:

$\mathbf{S}$*, the surface of interest;* ρ*, a density function defined on* $\mathbf{S}$*;*

k*, number of generators;* $\{\mathbf{z}_i\}_{i=1}^k$*, the initial set of generators.*

Output:

$\{V_i\}_{i=1}^k$*, a CCVT with k generators* $\{\mathbf{z}_i\}_{i=1}^k$ *in* $\mathbf{S}$.

Iteration:

1. *Construct the Voronoi tessellation* $\{V_i\}_{i=1}^k$ *of* $\mathbf{S}$ *with generators* $\{\mathbf{z}_i\}_{i=1}^k$.
2. *Take the constrained mass centroids of* $\{V_i\}_{i=1}^k$ *as the new set of generators* $\{\mathbf{z}_i\}_{i=1}^k$.
3. *Repeat the procedures* 1 *and* 2 *until some stopping criterion is met.*

It is clear that Algorithm 3.1 is almost identical to Algorithm 1.1 except the constrained mass centroids are used instead of standard mass centroids in step 2 of each iteration. So Algorithm 3.1 again can be regarded as a fixed point iteration of $\mathbf{T}$, the Lloyd map for CCVTs which now is defined to map the current generators to the constrained mass centroids of the corresponding Voronoi regions. It is transparent that the analysis done in sections 2.1 and 2.2 can be applied here, so we obtain the following general results similar to Theorems 2.3 and 2.5.

THEOREM 3.1. *Any limit point* $\mathbf{Z}$ *of the Lloyd algorithm for computing CCVTs is a fixed point of the Lloyd map for CCVTs, and thus,* $(\mathbf{Z}, \mathbf{Z})$ *is a stationary point of* $\mathcal{H}$*. Moreover, for an iteration started with a given initial guess, all elements in the set of its limit points share the same distortion value. Furthermore, if the set of fixed points with the same distortion value is finite, the Lloyd iteration for CCVTs converges globally.*

Now suppose that $\mathbf{S}$ is a smooth curve without self-intersection such as $\mathbf{S} = f(\Omega)$, where $\Omega = [a, b]$ for some smooth function f; then using the analysis similar to that provided in section 2.3, we obtain the following result.

THEOREM 3.2. *The Lloyd algorithm for computing CCVTs of* $\mathbf{S}$ *is globally convergent for any positive and smooth density function when* $\mathbf{S}$ *is a bounded smooth curve.*

Note that, unlike the one-dimensional conventional CVT in $\mathbb{R}^1$, we have not given any general estimate here on the convergence rate of the Lloyd algorithm for CCVTs. Even for the case where $\mathbf{S}$ is a bounded smooth curve, the geometric convergence rate has not been carefully derived, though the notion of contraction for the Lloyd map has been studied for density functions which share similar logarithmic concave properties with respect to the angular variable in the case of a perfect disc [12]. There are also natural generalizations of the Lloyd algorithm to the anisotropic CVTs as defined in [16] and also [18]. The details are omitted here.

4. Numerical examples. To further substantiate some of our earlier analysis, we now present a few numerical examples. All examples given below correspond to the Lloyd iteration on the interval $[0, 1]$.

4.1. Constant density. In Figure 2, we show a log-log plot of both the numerical estimates and the analytical estimate $1 - ||\mathbf{dT}|| \sim \pi^2/(4k^2)$ with respect to the constant density for various values of k, the number of generating points. The two estimates match very well and the results verify that the analytical estimates are very sharp.

4.2. Nonconstant density. Consider the case of $\rho(x) = e^{-x^2}$. Figure 3 compares the analytical estimate with the computed norms of the Jacobian for different system sizes. Here, the analytical estimate is based on $c_1^2 k^{-2}$ with the constant c_1 estimated by (2.14) with $c_0 = \sqrt{2/e}$, $M = 1$, and $\int_0^1 \rho^{1/3}(x)dx = \sqrt{3\pi} \cdot \mathrm{Erf}(1/\sqrt{3})/2$, which leads to $c_1 = \sqrt{\pi} \cdot \mathrm{Erf}(1/\sqrt{3})/2e \sim 0.19$. The plot is again given in log-log scale, and we see that although we underestimated the exact value of c_1, the slope was equal to -2 for both estimates, which indicates good agreement of the asymptotic rates on the order of $1 - O(1/k^2)$.

Figure 4 gives a similar comparison for $\rho(x) = 1 + x^4 \cos(\pi x)$. The numerical data in this case were compared to the asymptotic rate of $1 - \pi^2/4k^2$.

Figures 5–7 provide some insight into the dependence of the actual convergence factor on the number of generators and on the density function. The convergence factor in the plot is defined as the ratio of the 2-norm defects between two consecutive iterations after sufficiently many steps. A density function of the form $\rho(x) = 1 + \epsilon \cos^2(\pi x)$ is chosen. In Figure 5, we fix the number of generators to be $k = 16$, while letting ϵ vary in the range $[10^{-10}, 10^{10}]$. It is seen that the actual convergence factor and the theoretical estimate given by $||\mathbf{dT}||$ agree well in general.

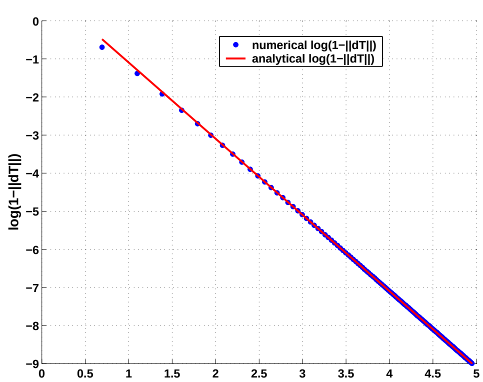

FIG. 2. *Convergence of Lloyd method for constant density.*

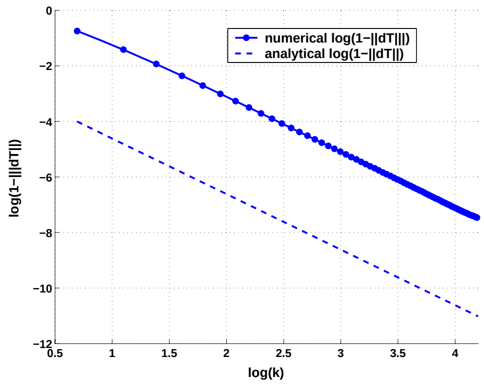

FIG. 3. *Convergence factor of Lloyd method for* $\rho(x) = e^{-x^2}$.

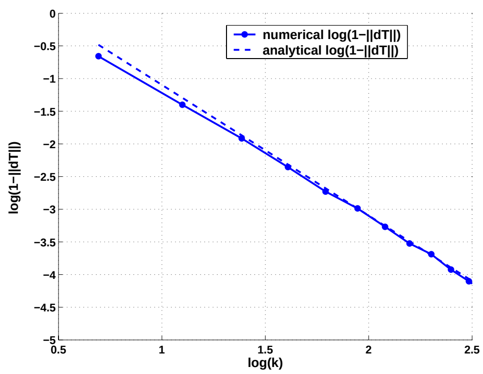

FIG. 4. *Convergence factor of Lloyd method for* $\rho(x) = 1 + x^4 \cos(\pi x)$.

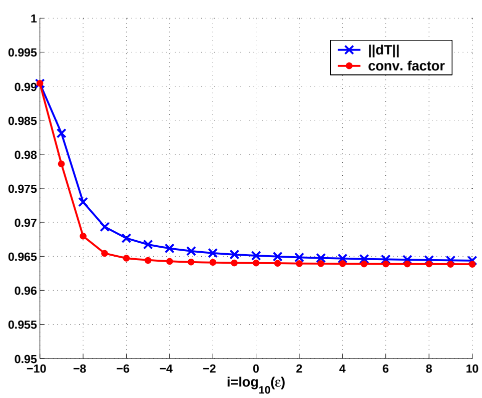

FIG. 5. *Convergence factor for* $k = 16$ *and* $\rho(x) = 1 + \epsilon \cos^2(\pi x)$ *with* $\epsilon = 10^{-10} : 10^{10}$.

To see the effect of the increasing k, in Figure 6 we fix ϵ and let the number of generators vary. The two estimates again compare well with each other.

To see more clearly the dependence of convergence rates on k, we again plot the data in a log-log scale for the density $\rho(x) = 1 + 10^3 \cos^2(\pi x)$ against the number of generators. The slope value of -2 is very evident from Figure 7, which is consistent with our earlier analysis.

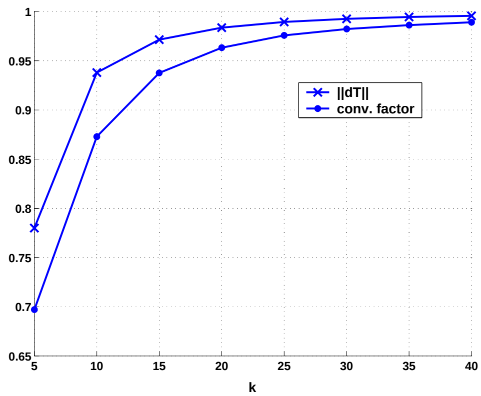

FIG. 6. *Convergence factor for* $\rho(x) = 1 + 10^3 \cos^2(\pi x)$ *and* $k = 2 : 40$.

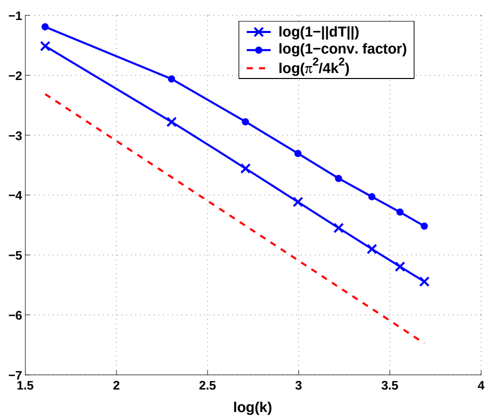

FIG. 7. *Asymptotic behavior of the convergence factor for* $\rho(x) = 1 + 10^3 \cos^2(\pi x)$.

5. Conclusions. In many practical applications of the centroidal Voronoi tessellations, it is very important to find their reliable and efficient constructions. Lloyd algorithm has been one of the most widely used techniques for such purposes. In this paper, a systematic study of both the local and the global convergence properties of the Lloyd algorithm is presented. We established several new convergence theorems, made further characterizations on the properties of the iteration, and performed relevant numerical experiments. We also extended our discussion to more general settings such as the construction of the CCVTs on a manifold. Still, one important open problem remains, that is, the global convergence of the Lloyd algorithm in any dimensions for any smooth density. The nondegeneracy of the Lloyd map should be true in this general case, but its proof has not been produced rigorously except for the one-dimensional case discussed here. We hope that our present study generates some interest along this direction, as there are certainly many issues to be considered further—in particular, the improvement of the Lloyd method for large number of generators. Even in the one-dimensional case, both our theoretical estimates and the experiments indicate the possible slow convergence rates. Recently, we have worked on making improvements in two directions: one is to explore the coupling with Newton-like methods, and another is to introduce the ideas of multilevel schemes [5, 6, 20]. As previously studied in [30], one may also consider parallel implementation issues for these approaches. In conclusion, there are still many interesting problems associated with the construction of CVTs that can be investigated in the future.

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