Computation of Centroidal Voronoi Tessellations in High Dimensional Spaces

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Abstract—**Owing to the natural interpretation and various desirable mathematical properties, centroidal Voronoi tessellations (CVTs) have found a wide range of applications and correspondingly a vast development in their literature. However, the computation of CVTs in higher dimensional spaces remains difficult. In this letter, we exploit the non-uniqueness of CVTs in higher dimensional spaces for their computation. We construct such high dimensional tessellations by decomposing into CVTs in one-dimensional spaces. We then prove that such a tessellation is centroidal under the condition of independence among densities over the 1-D spaces. Various numerical evaluations backup the theoretical result through the low energy of the grid-like tessellations, and are obtained with minimal computation time. We also compare the proposed decomposition method with the popular MacQueen's probabilistic method.**

Index Terms—**Centroidal voronoi tessellations, computational methods, high-dimensional spaces.**

I. INTRODUCTION

VORONOI diagram is a partition of a set into subsets containing elements that are close to each other according to a certain metric. Even though they date centuries, Voronoi tessellations (VTs) have been immensely helpful in various applications ranging from health to computer graphics to natural sciences. The first documented application of VTs appeared in [1] on the 1854 cholera epidemic in London in which it is demonstrated that proximity to a particular well was strongly correlated to deaths due to the disease [2]. In more recent decades, VTs have almost become a common basis tool for path planning algorithms by multi-robot systems in the field of coverage control [3] to such an extent that the VT-based coverage control has been generalized using optimal transport-based control [4]. An adaptive coverage controller is proposed in [5] where the leader in the leader-follower strategy therein distributes the followers within its obstacle-free sensing range, and the optimized distribution is obtained through CVT.

In their study on optimality of multi-robot coverage control, the authors in [6] draw a relationship between CVT configurations and the sufficient condition for optimality through the spatial derivative of the density.

In line with the popularity of CVTs, remarkable amount of contributions have been made to further their development. Reference [7] refines the notion of Constrained CVTs and derives various properties like their characterization as energy minimizers. Focusing on 1-D Voronoi diagrams, [8] develops an optimal algorithm for computing collinear weighted Voronoi diagrams that is conceptually simple and attractive for practical implementations. Reference [9] studies the inverse Voronoi problem in-depth.

Despite the wide applicability and vast development in the literature pertaining to CVTs, there remain challenges and open questions, especially in high dimensional spaces. For dimensions greater than one, rigorously verifying that a given CVT is a local minimum can prove difficult, for example [10] uses variational techniques to give a full characterization of the second variation of a CVT and provides sufficient conditions for a CVT to be a local minimum. Moreover, in high dimensional spaces, the number of CVTs under certain conditions and their quality is elusive, and their computation remains difficult.

In this letter, we employ CVTs in 1-D spaces to construct a tessellation in a higher dimensional space. Then we prove that such a tessellation is a CVT in the higher dimensional space under certain conditions. Such a construction is a simple and yet a powerful technique that is guaranteed to render at least one of the many non-unique CVTs in high dimensions in a fast and efficient way with minimal computational requirements.

The desired number of centroids in the higher dimensional space is a product of the number of centroids in the 1-D spaces, and we consider dimensions in the orders of ten. Accordingly, if the dimension is too large, one can limit the number of centroids in 1-D spaces in order to keep the total number of centroids meaningful. Doing so also has the advantages of further reduction in computational time.

This letter is structured as follows. In Section II we formally define CVTs, discuss their uniqueness properties, and existing methods to compute them. In Section III we construct a tessellation in a higher dimensional space and prove that it is also a CVT. In Section IV we provide numerical results of CVTs under different conditions, and compare with MacQueen's probabilistic method. Finally, we present some conclusions and remark on future work in Section V.
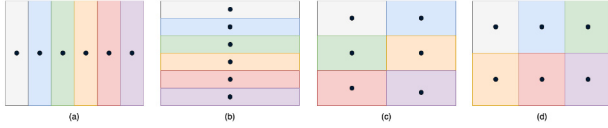
Fig. 1. CVT is not necessarily unique in $\mathbb{R}^2$. Voronoi regions are shown in different colors while their centroids are marked as black dots.

II. PRELIMINARIES

Consider a region $\Omega \subset \mathbb{R}^n$, $n \geq 1$. Let $N \in \mathbb{N}$, $V_i \subset \Omega$, $\forall i \in I_N$, and denote index set as $I_N = \{1, 2, \ldots, N\}$. Let $\rho(.)$ denote a measure of information or the probability density over Ω.

1 Tessellation: $\{V_i\}_{i \in I_N}$ is a tessellation of Ω if $V_i \cap V_j = \emptyset$ for $i \neq j$, and $\cup_{i \in I} V_i = \Omega$.

2 Voronoi region and generators: The Voronoi region V_{z_i} of the Voronoi generator z_i is $V_{z_i} = \{x \in \Omega : \|x - z_i\| < \|x - z_j\|, \ i \neq j$ and $i, j \in I_N\}$.

3 Voronoi tessellation: The set of Voronoi regions $\mathbf{V_z} = \{V_{z_i}\}_{i \in I_N}$ of $\{z_i\}_{i \in I_N}$ is called a VT: $\{\mathbf{z}, \mathbf{V_z}\}$.

The mass centroid of a region $V_i \subset \Omega$ under the probability density function $\rho(.)$ is defined as:

$$z_{V_i, \rho}^c = \frac{\int_{V_i} x \rho(x) dx}{\int_{V_i} \rho(x) dx} \qquad (1)$$

A VT in which the generators are the mass centroids of their respective Voronoi regions is called a *Centroidal Voronoi Tessellation* (CVT), [11].

A. Uniqueness of CVT

Given a region $\Omega \subset \mathbb{R}^n$, a positive integer N, and a density function $\rho(x)$ on Ω, the minimizer of the following functional is a CVT, [11]:

$$\mathcal{K}((z_i), i \in I_N) = \sum_{i \in I_N} \int_{x \in V_{z_i}} \rho(x) \|x - z_i\|^2 dx \qquad (2)$$

Also referred to as the energy of the tessellation, $\mathcal{K}$ is continuous, it possesses a global minimum, and may have local minimizers, [11]. It is showed in [12] that the solution of (2) is unique in 1-D regions with a logarithmically concave continuous probability density function of finite second moment. As reiterated in [10], for $n = 1$, the logarithmic concavity condition implies that any CVT is a local minimum, and further, that there is a unique CVT that is both a local and a global minimum of $\mathcal{K}(\mathbf{z})$, where $\mathbf{z} = \{z_i\}_{i \in I_N}$. While the conditions for uniqueness of vector quantizers without any assumptions on the region, density or the number of quantizers N, remains an open area of research, it is proved in [10] that for $N = 2$, there does not exist a unique CVT for any density for $n > 1$.

For a graphic illustration on non-uniqueness of CVTs, consider a rectangle in $\mathbb{R}^2$ with six generator points under Uniform distribution. As shown in Fig. 1, there are multiple CVTs: all the four VTs shown are centroidal, and additional CVTs can be obtained through rotations.

B. Computation of CVT in 1-D Regions

Given a region $\Omega \subset \mathbb{R}$, a number of generators N, and a density function $\rho(x)$ over Ω, there are various algorithms to compute a CVT in Ω; the deterministic Lloyd's algorithm being the most popular. Introduced in [13] to find the optimal quantization in pulse-code modulation, at the core of it, Lloyd's algorithm is an iteration between constructing VTs and their centroids.

Another method to obtain a CVT in 1-D is through the system of nonlinear equations (SNLE). The core idea is to parameterize the Voronoi regions in terms of their centroids: $V_i = [\frac{z_{i-1} + z_i}{2}, \frac{z_i + z_{i+1}}{2}], \forall i \in I_N$. The mass centroids from (1), with $z_{V_i, \rho}^c$ denoted as z_i^c for ease of notation, can then be written in terms of the parameterized regions:

$$z_i^c = \frac{\int_{\frac{z_{i-1}^c + z_i^c}{2}}^{\frac{z_i^c + z_{i+1}^c}{2}} x \rho(x) dx}{\int_{\frac{z_{i-1}^c + z_i^c}{2}}^{\frac{z_i^c + z_{i+1}^c}{2}} \rho(x) dx} \qquad (3)$$

Writing (3) for all the centroids results in N equations and N number of unknowns: z_i^c's. This is the SNLE, whose solution is the set of centroids of the CVT. In 1-D regions, the centroids are directly used to define the corresponding Voronoi partitions.

While the deterministic Lloyd's algorithm and analytical SNLE obtain the CVT in a deterministic way, MacQueen's method developed in [14] takes a probabilistic approach. However, the computation of CVT in higher dimensional spaces still remains a challenge. Reference [15] considers parallel implementations of Lloyd's, MacQueen's and a method developed therein, and presents the CVT results for regions up to two dimensions while noting that the method can be extended to higher dimensions. Although [16] results in faster convergence to a CVT, it does not easily extend to higher dimensions.

Most CVT computation methods provide the CVT centroids but not the partitions or the tessellation energy. While in 1-D spaces, it is straight-forward to obtain the complete tessellations from the centroids, such extension is difficult, if not impossible, for arbitrary dimensional spaces. The lack of complete information about the tessellation and their qualities, for example through their energies, limits the existing computational methods. In the next Section, we present a way to obtain a higher dimensional CVT by decomposing it into a series of CVTs in 1-D spaces.

III. COMPUTATION OF CVT IN HIGHER DIMENSIONS

In this Section, we first propose a simple method to obtain a tessellation in any higher dimensional space from CVTs in 1-D spaces. Then, we present the proof that a tessellation constructed in such a way is also a CVT.

Consider a region $\Omega \subset \mathbb{R}^n$, $n > 1$, and $\Omega = \Omega_1 \times \Omega_2 \times \ldots \times \Omega_n$. Let $\rho(.)$ be the probability density function over Ω, and $\rho_i(.)$ be the density function over Ω_i, $\forall i \in I_n = \{1, 2, \ldots, n\}$. That is, $\rho(.)$ is the joint density, and $\{\rho_i(.)\}_{i \in I_n}$ are the marginal densities.

Let the number of generators in a CVT of Ω_i under $\rho_i(.)$ be N_i, and let the number of generators in a CVT of Ω under $\rho(.)$ be N, where $N = N_1 \times \ldots \times N_n$. Denote a CVT in Ω_i as $\{\mathbf{z}_i^*, \mathbf{V}_{\mathbf{z}_i^*}\}$. Here, $\mathbf{z}_i^* = \{z_{i,j}^*\}_{j \in I_{N_i}}$ is the set of all the centroids of the CVT in Ω_i, and $\mathbf{V}_{\mathbf{z}_i^*} = \{V_{z_{i,j}^*}\}_{j \in I_{N_i}}$ is the set of their respective Voronoi regions. Similarly, denote a CVT in Ω as $\{\mathbf{z}^*, \mathbf{V}_{\mathbf{z}^*}\}$, where $\mathbf{z}^* = \{z_k^*\}_{k \in I_N}$ denotes the centroids, $\mathbf{V}_{\mathbf{z}^*} = \{V_{z_k^*}\}_{k \in I_N}$ denotes their corresponding Voronoi regions.

The set of centroids in Ω can be given as a matrix $\mathbf{z}^* = [z_1^* \, z_2^* \ldots z_N^*] \in \mathbb{R}^{n \times N}$, where each matrix column $\{z_k^*\}_{k \in I_N} \in \mathbb{R}^n$ denotes a centroid in $\mathbb{R}^n$. Similarly, the set of centroids in Ω_i is given as a vector $\mathbf{z}_i^* = [z_{i,1}^* \, z_{i,2}^* \ldots z_{i,N_i}^*] \in \mathbb{R}^{N_i}$, where each element is a centroid in $\mathbb{R}$. Additionally, note that $V_{z_k^*} \subset \mathbb{R}^n$ while $V_{z_{i,j}^*} \subset \mathbb{R}$.

Let $I_{n \times N}$ denote the matrix containing all combinations of vectors $I_{N_i}, \forall i \in I_n$. That is, define the kth of the N columns of $I_{n \times N}$ as $\{[j_1 \, j_2 \ldots j_n]^T$ such that $j_i \in I_{N_i}, \ i \in I_n\}$ For example, if $n = 2, N_1 = 2, N_2 = 3$, then $N = 2 \times 3 = 6$ and

$$I_{n \times N} = \begin{bmatrix} 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 2 & 3 & 1 & 2 & 3 \end{bmatrix} \tag{4}$$

With all the notations defined, we now present a straightforward method of constructing a tessellation in Ω from CVTs in $\Omega_i's$.

Tessellation construction in Ω

For each dimension $i \in I_n$, construct a CVT in Ω_i: $\{\mathbf{z}_i^*, \mathbf{V}_{\mathbf{z}_i^*}\}$

Obtain the n coordinates of each centroid in Ω and its Voronoi region as:
$\forall k \in I_N$:
  $\forall i \in I_n$:
    $z_k^*(i) = z_{I_{n \times N}(i,k)}^*$
    $V_{z_k^*} = V_{z_{I_{n \times N}(i,k)}^*}$
The set of all the centroids $\{z_k^*\}_{k \in I_N}$ and their Voronoi regions $\{V_{z_k^*}\}_{k \in I_N}$ make the tessellation in Ω: $\{\mathbf{z}^*, \mathbf{V}_{\mathbf{z}^*}\}$

Having obtained the tessellation, we show in the following theorem that $\{\mathbf{z}^*, \mathbf{V}_{\mathbf{z}^*}\}$ constructed from $\{\mathbf{z}_i^*, \mathbf{V}_{\mathbf{z}_i^*}\}_{i \in I_n}$ is a CVT in Ω.

Theorem: Let $\Omega = \Omega_1 \times \Omega_2 \times \ldots \times \Omega_n \subset \mathbb{R}^n, n > 1$. Let $\rho(.)$ be the joint density function over Ω, and $\rho_i(.)$ be the density function over $\Omega_i, \forall i \in I_n$. If $\rho(x_1, \ldots, x_n) = \prod_{i \in I_n} \rho_i(x_i)$, then $\forall i \in I_n, \forall k \in I_N$ and $k_i = I_{n \times N}(i, k)$, we have:

$$z_k^* = (z_{1,k_1}^*, \ z_{2,k_2}^*, \ldots, z_{n,k_n}^*) \tag{5}$$
$$V_{z_k^*} = V_{z_{1,k_1}^*} \times V_{z_{2,k_2}^*} \times \ldots \times V_{z_{n,k_n}^*}. \tag{6}$$

Proof: Consider $x \in V_{z_{1,k_1}^*} \times \ldots \times V_{z_{n,k_n}^*}, \forall i \in I_n$, and denote $x = (x_1, \ldots, x_n)$. Because V_{z_{i,k_i}^*} is the Voronoi region of z_{i,k_i}^*, $\forall i \in I_n$, we have for any $j_i \in I_{N_i}$:

$$\|x_i - z_{i,k_i}^*\|_2 \le \|x_i - z_{i,j_i}^*\|_2$$
$$\implies (x_i - z_{i,k_i}^*)^2 \le (x_i - z_{i,j_i}^*)^2 \tag{7}$$

Summing (7) $\forall i \in I_n$,

$$(x_1 - z_{1,k_1}^*)^2 + \ldots + (x_n - z_{n,k_n}^*)^2$$
$$\le (x_1 - z_{1,j_1}^*)^2 + \ldots + (x_n - z_{n,j_n}^*)^2$$

$$\implies \sqrt{((x_1 - z_{1,k_1}^*)^2 + \ldots + (x_n - z_{n,k_n}^*)^2)}$$
$$\le \sqrt{((x_1 - z_{1,j_1}^*)^2 + \ldots + (x_n - z_{n,j_n}^*)^2)}$$

Let $\hat{z}_k^* = (z_{1,k_1}^*, z_{2,k_2}^*, \ldots, z_{n,k_n}^*)$, then:

$$\|x - \hat{z}_k^*\|_2 \le \|x - z_j^*\|$$
$$\implies V_{\hat{z}_k^*} = V_{z_{1,k_1}^*} \times \ldots \times V_{z_{n,k_n}^*} \tag{8}$$

That is, $V_{z_{1,k_1}^*} \times \ldots \times V_{z_{n,k_1}^*}$ is the Voronoi region of $\hat{z}_k^*$.

Consider the ith coordinate of $\hat{z}_k^*$. Since z_{i,k_i}^* is the centroid of V_{z_{i,k_i}^*}, by definition of centroid, we have:

$$z_{i,k_i}^* = \frac{\int_{V_{z_{i,k_i}^*}} x_i \rho_1(x_i) dx_i}{\int_{V_{z_{i,k_i}^*}} \rho_n(x_i) dx_i}$$

$$= \frac{\int_{V_{z_{1,k_1}^*}} \rho_1(x_1) dx_1}{\int_{V_{z_{1,k_1}^*}} \rho_1(x_1) dx_1} \times \ldots \times \frac{\int_{V_{z_{i,k_i}^*}} x_i \rho_i(x_i) dx_i}{\int_{V_{z_{i,k_i}^*}} \rho_i(x_i) dx_i}$$

$$\times \ldots \frac{\int_{V_{z_{n,k_n}^*}} \rho_n(x_n) dx_n}{\int_{V_{z_{n,k_n}^*}} \rho_n(x_n) dx_n} \tag{9}$$

Because the events in Ω_i are independent of those in Ω_j, $\forall i \ne j, \ i, j \in I_n$, we have $\rho(x_1, \ldots, x_n) = \rho_1(x_1) \times \ldots \times \rho_n(x_n)$. Substituting this relation in (9) implies:

$$z_{i,k_i}^* = \frac{\int_{V_{z_{1,k_1}^*}} \ldots \int_{V_{z_{n,k_n}^*}} x_i \rho(x_1, \ldots, x_n) dx_1 \ldots dx_n}{\int_{V_{z_{1,k_1}^*}} \ldots \int_{V_{z_{n,k}^*}} \rho(x_1, \ldots, x_n) dx_1 \ldots dx_n}$$

which, by (1), is the ith coordinate of the kth of the N centroids – z_k^* – in Ω with density $\rho(.)$. That is, $z_k^*(i) = z_{i,k_i}^*$. Since this holds for all $i \in I_n$ coordinates, we have $z_k^* = \hat{z}_k^* = (z_{1,k_1}^*, z_{2,k_2}^*, \ldots, z_{n,k_n}^*)$, and hence proving (5). On the other hand, since $V_{z_{1,k_1}^*} \times \ldots \times V_{z_{n,k_1}^*}$ is the Voronoi region of $\hat{z}_k^*$ from (8), and $z_k^* = \hat{z}_k^*$, we have $V_{z_{1,k_1}^*} \times \ldots \times V_{z_{n,k_1}^*}$ is the Voronoi region of z_k^*, hence proving (5). Since this holds for all N centroids in Ω, we have that $\mathbf{V}_{\mathbf{z}^*} = \{V_{z_k^*}\}_{k \in I_N}$ is the Voronoi partition of $\mathbf{z}^* = \{z_k^*\}_{k \in I_N}$.

Having shown that $V_{z_{1,k_1}^*} \times \ldots \times V_{z_{n,k_1}^*}$ is the Voronoi region of $\hat{z}_k^*$ and that $\hat{z}_k^*$ is its centroid, we now show that $\{V_{z_k^*}\}_{k \in I_N}$ is a tessellation in Ω. Because $\mathbf{V}_{\mathbf{z}_i^*}$ is a tessellation in $\Omega_i, \forall i \in I_n$, we have:

$$\bigcup_{k \in I_N} \prod_{i \in I_n} V_{z_{i,k_i}^*} = \prod_{i \in I_n} \bigcup_{j_i \in I_{N_i}} V_{z_{i,j_i}^*} = \prod_{i \in I_n} \Omega_i = \Omega$$

$$\forall \, k \ne l, \ V_{z_k^*} \bigcap V_{z_l^*} = \prod_{i \in I_n} V_{z_{i,k_i}^*} \bigcap \prod_{i \in I_n} V_{z_{i,l_i}^*}$$
$$= \prod_{i \in I_n} (V_{z_{i,k_i}^*} \cap V_{z_{i,l_i}^*}) = \emptyset$$

Hence, $\{V_{z_k^*}\}_{k \in I_N}$ is a tessellation in Ω.

Since $\mathbf{z}^*$ are the centroids of partitions $\mathbf{V}_{\mathbf{z}^*}$, $\mathbf{V}_{\mathbf{z}^*} = \{V_{z_k^*}\}_{k \in I_N}$ are the Voronoi regions of $\mathbf{z}^*$, and $\{V_{z_k^*}\}_{k \in I_N}$ is a tessellation in Ω, we have that $\{\mathbf{z}^*, \mathbf{V}_{\mathbf{z}^*}\}$ is a CVT in Ω with density $\rho(.)$. ∎

Consider $\Omega = [0, 20] \times [0, 10]$ in $\mathbb{R}^2$ with density $\rho(.) \sim \mathcal{N}(\mu, \Sigma)$, where $\mu = (12, 7)$ and $\Sigma = [4 \ 0; 0 \ 1]$. Denote the
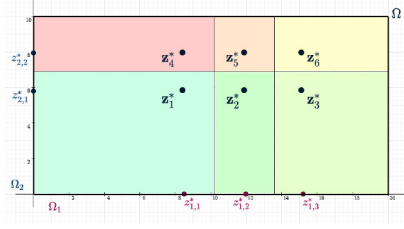
Fig. 2.   CVT in Ω with density $\mathcal{N}(\mu, \Sigma)$ where $\mu = [12; 7]$ and $\Sigma = [4\ 0; 0\ 1]$.

CVT as $\{\mathbf{z}^*, \mathbf{V}_{\mathbf{z}^*}\}$, where $\mathbf{z}^* = (z_1^*, \ldots, z_6^*)$, and $z_k^* \in \mathbb{R}^2, \forall k \in I_6 = \{1, \ldots, 6\}$.

On the other hand, let $N_1 = 3$ and $N_2 = 2$. Consider the unique CVT in $\Omega_1 = [0, 20]$ for $\rho_1(.) \sim \mathcal{N}(12, 4)$, which is denoted $\{\mathbf{z}_1^*, \mathbf{V}_{\mathbf{z}_1^*}\}$. Note $\mathbf{z}_1^* = (z_{1,1}^*, z_{1,2}^*, z_{1,3}^*)$, and $z_{1,j}^* \in \mathbb{R}, \forall j \in I_3$. Similarly, consider the unique CVT in $\Omega_2 = [0, 10]$ for $\rho_1(.) \sim \mathcal{N}(7, 1)$, which is denoted $\{\mathbf{z}_2^*, \mathbf{V}_{\mathbf{z}_2^*}\}$. Note $\mathbf{z}_2^* = (z_{2,1}^*, z_{1,2}^*)$, and $z_{1,j}^* \in \mathbb{R}, \forall j \in I_2$. These generators are shown in Fig. 2: the region Ω_1 and the CVT generators in it are showed in pink, and the region Ω_2 and the CVT generators in it are showed in blue.

Suppose $N_i = N$ and $N_j = 1$, $\forall j \neq i$ for some $i, j \in I_n$, $n > 1$. This corresponds to the case where all the centroids in $\mathbb{R}^n$ are "aligned" along the ith dimension, that is, the centroids only differ in their i^{th} coordinate. In such a case, the decomposition of obtaining the CVT in $\mathbb{R}^n$ into n CVTs in $\mathbb{R}$ is equivalent to obtaining a CVT in $\mathbb{R}$ with all other dimensions held constant. While the proposed method of obtaining a CVT in higher dimensions by employing a combination of CVTs in $\mathbb{R}$ does not result in every possible CVT of the higher dimension under the given conditions, we are guaranteed to obtain at least one of them in a straightforward manner with minimal computation.

IV. NUMERICAL RESULTS

In this Section, we present a set of numerical results to demonstrate the ease of extension in higher dimensions through the time required to compute the CVT and it's energy. Additionally, for 2 and 3 dimensional spaces we also present the tessellations graphically. To obtain the CVTs in 1-D spaces, one can employ Lloyd's algorithm or solve the system of nonlinear equations; the latter being more desirable when $N_i's$ are low.

We compare the proposed decomposition method to obtain a CVT in higher dimensional space with a popular probabilistic method – MacQueen's which was introduced in [14]. The elegant MacQueen's algorithm requires Monte Carlo sampling for initialization and randomization in every iteration to compute the centroids in a given space under certain density. Its performance vastly depends on the Monte Carlo samples, and accordingly on the method employed to generate such samples. The authors in [15] compare their proposed method to obtain a CVT with MacQueen's method for 1-D spaces and employ rejection sampling to obtain Monte Carlo samples. However, the rejection method does not readily scale to higher dimensions; its high rejection rate makes it extremely inefficient to generate Monte Carlo samples according to a desired distribution in a higher dimensional space [17]. Since our focus
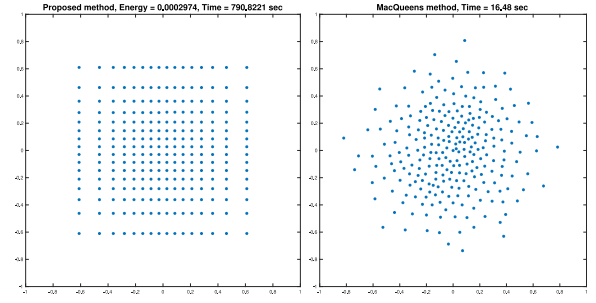

Fig. 3.   CVT of 256 centroids under $\rho_1(x_1) = \rho_2(x_2) = e^{-10x^2}$.

is CVT in high-dimensional spaces, we employ Metropolis-Hasting algorithm [17] to obtain the Monte Carlo samples for MacQueen's method. The termination criteria we employ for implementation of MacQueen's is the change in the norm of the centroids over each update; if the norm changes less than 10^{-6} we terminate the MacQueen's iterations.

Additionally, [15] compares their results with those from MacQueen's through the CVT energy for 1-D spaces and graphically for two-dimensional spaces. While obtaining the Voronoi partitions is very straight-forward in 1-D spaces, its computation in higher dimensions is difficult. The requirement of the knowledge of Voronoi cell boundary of each centroid along with the computation of the cell energy, which involves the computation of "area" of arbitrary high-dimensional polygons, makes the computation of the tessellation energy in high dimensional spaces very difficult. Therefore, following [15] we compare our results with those from MacQueen's visually in two and three dimensions, and through computation time in higher dimensional spaces.

Consider $\Omega = [-1, 1] \times [-1, 1]$. Following the cases taken up in [15], we let the density function over Ω be e^{-10x^2}. The CVT with 16 centroids in each dimension, obtained using the proposed decomposition method and the MacQueen's method are shown in Fig. 3. As designed and expected, the tessellation from the decomposition has a well drawn out grid-like structure with the intensity of centroids being higher in the center of Ω. The resulting tessellation is a CVT with (low) energy of 2.9×10^{-4} and was obtained in computational time as less as 13.18 minutes in an ordinary laptop – MacBook Air 2015 with 2.2 GHz Dual-Core Intel Core i7.

Next case of demonstration is in the region $\Omega = [0, 20] \times [0, 20]$ with density $\mathcal{N}(\mu, \Sigma)$, where $\mu = (5, 6.5)$ and $\Sigma = [2\ 0; 0\ 1]$. The resulting CVTs with 3000 centroids, obtained using the proposed method and the MacQueen's method are shown in Fig. 4.

Moving to 3 dimensional spaces, we consider $\Omega = [0, 10] \times [0, 10] \times [0, 10]$ with density $\mathcal{N}(\mu, \Sigma)$, where $\mu = (6, 5, 3.5)$ and $\Sigma = [2\ 0\ 0; 0\ 1\ 0; 0\ 0\ 1]$. The resulting well-aligned grid-like CVT with 16 centroids in each dimension, with energy 0.1616, is shown in Fig. 5. In contrast to the aligned CVT, the solution tessellation from MacQueen's under the same conditions is also shown in Fig. 5.

The convergence of the MacQueen's iterates to a CVT is not guaranteed for all conditions, and due to it's probabilistic nature, it's performance vastly depends on the Monte Carlo
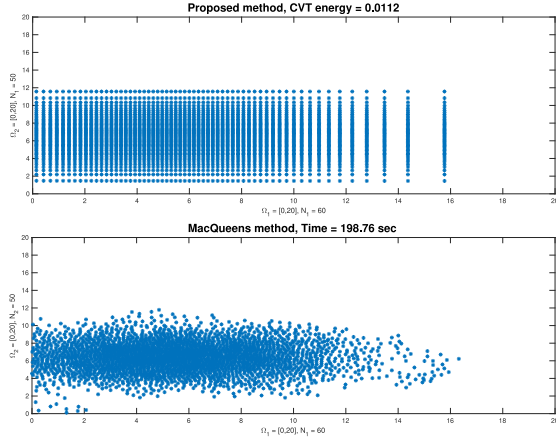
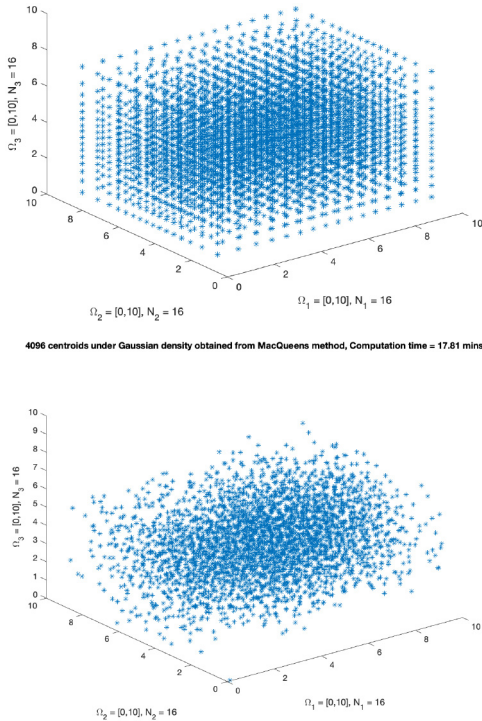Fig. 4.   CVT of 3000 centroids with Gaussian density.

Fig. 5.   Scalability and generalizability to any density: CVT of 4096 centroids under Gaussian density.

TABLE I
PROPOSED METHOD FOR $\Omega_i = [-1, 1], \forall i \in I_n$ UNDER e^{-10x^2}. NOTE THE ABSENCE OF CVT ENERGY FROM MACQUEEN'S

n	$N = \prod_i N_i$	CVT energy $\times 10^{-3}$	Time (min)	MacQueen's time (min)
4	$4096 = 8^4$	0.68	6.174	2.644
5	$4096 = 4^3 \times 8^2$	1.2	4.248	1.433
8	$6561 = 3^8$	0.74	0.641	1.556
12	$4096 = 2^{12}$	0.21	0.480	1.425

the density function is through the Monte Carlo samples, our results have higher computation time than MacQueen's. We must note here that while we employ Lloyd's to obtain CVTs in 1-D spaces, one could employ MacQueen's or other CVT computation methods for the decomposed CVT in 1-D.

One of the areas where higher dimensional CVTs have found an application is in the field of evolutionary optimization. Recently introduced, MAP-elites [18] is an algorithm that illuminates search spaces in evolutionary optimization, allowing researchers to understand how interesting attributes of solutions combine to affect performance. To scale up the MAP-elites algorithm, authors in [19] employ CVTs, and therein, following [15], they employ MacQueen's method to obtain the CVTs and show the sufficiency of using 5000 centroids. In line with their result, we keep the total number of centroids in our results of high-dimensional CVTs, around the same. Similar to illuminating search spaces using MAP-elites, CVTs have been useful in the field of fluid dynamics and control through their role in finite-element analysis for discretization in space dimensions [20]. While the authors in [20] use CVT-based clustering for reduced-order modeling under uniform density, one could employ CVTs to model the underlying space according to candidate density functions. Specifically in such space discretization applications, the proposed method allows us a clear insight into the underlying solution (or search) space by evaluating all possible grid-like CVTs under any density function. For example, by varying the number of centroids per dimension we can obtain a number of different tessellations, and although this would not be exhaustive and there will still be more (non grid-like) CVTs under the same conditions, we can get a better idea about the solutions at different points in the underlying space through the energies of all the grid-like CVTs obtained from the proposed method.

In our last block of presentation of numerical results, we consider dimensions higher than 3 and vary $N_i, \forall i \in I_n$ such that $N = \prod_i N_i$ is around 5000. The corresponding results are given in Table I where we see that the computation time decreases with the increase in dimension n. This is because with increasing n, we decrease N_i to keep N around 5000. Hence, the computation of CVT in 1-D spaces with fewer centroids is faster. The low energy of all the tessellations is also worth noting. On the other hand, the computation time required to compute the centroids using MacQueen's method are lower but the solutions are opaque since it is difficult to evaluate their quality through their tessellation energy.

While the proposed method allows us to obtain a number of CVTs and their energies in a straight-forward fashion, it suffers

samples. Since we employ the deterministic Lloyd's method to compute the CVTs in one dimensional spaces for which convergence is proven, the proposed algorithm converges to a CVT without the performance being vastly tied to the initial samples. Moreover, our proposed decomposition method also provides deep insight into the tessellation (and hence the application in hand that requires the CVT) by allowing evaluation of the quality of all the solutions (CVTs) through their energies. This is because we decompose our high dimensional spaces into a series of 1-D spaces for which the Voronoi partitions, and hence the tessellation energy, are readily obtained. However, since Lloyd's computes the mass centroids at each iteration while in MacQueen's the only characterization of

from the curse of dimensionality. Considering 32 dimensions and 2 centroids per dimension, the problem requirement scales to a total of 2^{32} centroids. While the maximum array size allocated varies by the program and the software, such exponential growth in the number of centroids practically limits the proposed method to under 30 dimensions. However, the applications where the proposed decomposition method would be most beneficial do not require dimensions in hundreds. For example, the number of features in MAP-elites are typically less than 10; in [21] the authors consider a four-dimensional problem. Exploration of the solution space using finite element analysis is in space dimensions. In such applications the proposed method provides insightful tessellations at various markers in the solution space even for finer discretizations.

V. CONCLUSION

In order to fully rank the quality of all the CVTs under a certain higher dimensional space (read fixed region, number of centroids, and density), the knowledge of all the CVTs and their tessellation energy is required. However, the problem in such a comparison is the difficulty in obtaining CVTs in higher dimension spaces. Nevertheless, the tessellations constructed from CVTs in 1-D spaces, that appear to be well drawn out grid-like structures, are proved to be one of the many CVTs in such spaces of dimensions greater than 1. Hence, we are guaranteed to obtain at least one of the many non-unique CVTs in the higher dimensional space.

Additionally, as seen in the numerical results, the tessellation energy of such CVTs is quantifiably low and are obtained with minimal computational requirement. The proposed decomposition method does not make specific assumptions on the density function, it is scalable to a large number of centroids, and is flexible in terms of dimensions and discretization over each dimension. Owing to the same decomposition that makes it straight-forward to compute Voronoi cells in one-dimension and accordingly the tessellation energy, the proposed method also allows for insight into the system through the analysis of the quality of solutions using the tessellations' energies.

However, the (only) key assumption in the construction of CVTs in higher dimensional spaces from CVTs in 1-D spaces is the independence of the densities of the latter spaces. This limits the applicability of the developed idea in areas where CVTs are constrained to a surface, say computing CVT on a sphere, and will be a point of investigation for our future work. [Source code]

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