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PERIODIC CENTROIDAL VORONOI TESSELLATIONS

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Abstract. Centroidal Voronoi tessellations (CVTs) are Voronoi tessellations whose generators coincide with the mass centroids of the respective Voronoi regions. CVTs have become useful tools in many application domains of arts, sciences and engineering. In this work, for the first time the concept of the periodic centroidal Voronoi tessellations (PCVTs) - CVTs that exhibit certain periodicity properties in the Euclidean space - is introduced and given a rigorous treatment. We discuss the basic mathematical structures of the PCVTs and show how they are related to the so-called CVT clustering energy. We demonstrate by means of a concrete example that the clustering energy can lose smoothness at degenerate points which disproves earlier conjectures about the CVT energy being globally C^2-smooth. We discuss a number of algorithms for the computation of PCVTs, including modifications of the celebrated Lloyd algorithm and a recently developed algorithm based on the shrinking dimer dynamics for saddle point search. As an application, we present a catalog of numerically computed PCVT patterns for the two dimensional case with a constant density and a square unit cell. Examples are given to demonstrate that our algorithms are capable of effectively probing the energy surface and produce improved patterns that may be used for optimal materials design. The numerical results also illustrate the intrinsic complexity associated with the CVT energy landscape and the rich geometry and symmetry represented by the underlying PCVTs.

Key words. Centroidal Voronoi Tessellations, Periodic Centroidal Voronoi Tessellations, Clustering energy, Critical point, Saddle point, Lloyd's algorithm, Shrinking dimer dynamics, Complex energy landscape, Optimal material design.

1. Introduction

Centroidal Voronoi tessellations (CVTs) are Voronoi tessellations whose generators coincide with the mass centroids of the respective Voronoi regions [13]. Given their obvious geometric meaning, CVTs can be naturally viewed as a model and method for point distributions and spacial tessellations of regions/volumes in $\mathbb{R}^d$. Yet, they have also been generalized to many other spaces and abstract settings. Since the first comprehensive study on the subject published over a decade ago [13], the generality and universality of CVTs have turned them them into a widely applicable tool in many subjects of science and engineering such as image processing and analysis, vector quantization and data analysis, resource optimization, optimal placement of sensors and actuators for control, mobile sensing networks, logistics system, cell biology and territorial behavior of animals, phyllotaxis, geophysical flows, optimal materials design, model reduction, point sampling, numerical quadrature, mesh generation and optimization, meshless computing, and numerical partial differential equations, see for instance, [1, 4, 5, 7, 9, 13, 14, 15, 17, 18, 21, 25, 29, 34, 36, 37, 40, 45, 46]. At the same time, there has been much progress toward the development of efficient algorithms for the computation of CVTs [10, 11, 12, 13]. For a recent review on the subject, we refer to [16] where one may also find a more up-to-date list of references.

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In this work, we consider a special type of CVTs in the Euclidean space, namely, the periodic centroidal Voronoi tessellations (PCVTs). These special CVTs satisfy certain additional properties that make them periodic in space with respect to some unit cell. A rigorous definition and some of the related mathematical properties are given later, together with some discussions on the computation of PCVTs. It is easy to see that much of the general theory and algorithms developed for CVTs can be applied to PCVTs. For example, after some necessary modifications, an energy functional (which is often the CVT energy or the clustering energy) can be defined so that its critical points correspond to PCVTs. Such an energy functional has played an important role in the computation of CVTs, as it helps turning the computation of CVTs into a problem of nonlinear optimization. Indeed, for general CVTs, it is well-known that they correspond to critical points of the associated CVT clustering energy.

Our studies of PCVTs in the Euclidean space are motivated by a number of considerations. On one hand, with the spatial periodicity, PCVTs may have independent interests such as in the *latinized* CVT design [42] and in materials design that can take advantage of the symmetry and periodicity [43]. PCVTs also provide good examples to understand the interplay of geometry and symmetry in determining the energy landscape of the CVT clustering energy both near equilibrium states and near metastable or unstable transition states. Indeed, except in very special cases [33], the CVT energy is not convex in general. While the local equilibria of the energy are often of interest in most applications, the saddle points provide useful information on the energy barriers and the transition path. In fact, such saddle points might correspond to local minimizers of the energy subject to certain constraints. On the other hand, PCVTs are closely related to CVTs in the conventional sense as defined in [13]. In fact, according to the well-known Gersho's conjecture, one may speculate that as the number of generators gets large, locally all CVTs minimizing the energy would exhibit self-similar and periodic structures associated with the basic optimal Voronoi cells [26]. In two dimension, it was shown that such a cell is a regular hexagon [38] which is space tiling and forms a special PCVT in $\mathbb{R}^2$. The dual Delaunay triangulation leads to the tessellation formed by regular triangles which also serves as an optimal triangulation by many criteria. In three dimension, compelling numerical evidence also supports the conjecture [19] with the basic cell given by the truncated dodecahedron and the corresponding CVT forming a BCC lattice, which is again a special PCVT in $\mathbb{R}^3$. The dual triangulation is formed by the so called Sommerville tetrahedron which is understandably different from the regular tetrahedron as the latter is not space tiling. In addition to the facts mentioned above, the popular lattice based quantizer design [3] also leads to PCVTs corresponding to a constant density.

All of the above provides sufficient motivation for us to undertake a study of the periodic CVTs and their properties, which is the focus of this work. The paper is organized as follows. In Section 2 we formalize the concept of PCVT, illustrate them with several examples and relate them to the regular CVTs by means of the corresponding energy functional. Section 3 contains the discussion about the algorithms suitable construct PCVTs and motivates the choice of a modification of the Shrinking Dimer Dynamics algorithm as a method of choice for this problem. We also discuss the question of energy smoothness and provide a counterexample showing that the energy can fail to be smooth at a degenerate point. We move on to provide a list of examples showing the local equilibria and saddle points of the