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Truncated Newton-Based Multigrid Algorithm for Centroidal Voronoi Diagram Calculation

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Abstract. In a variety of modern applications there arises a need to tessellate the domain into representative regions, called Voronoi cells. A particular type of such tessellations, called centroidal Voronoi tessellations or CVTs, are in big demand due to their optimality properties important for many applications. The availability of fast and reliable algorithms for their construction is crucial for their successful use in practical settings. This paper introduces a new multigrid algorithm for constructing CVTs that is based on the MG/Opt algorithm that was originally designed to solve large nonlinear optimization problems. Uniform convergence of the new method and its speedup comparing to existing techniques are demonstrated for linear and nonlinear densities for several 1d and 2d problems, and $O(k)$ complexity estimation is provided for a problem with k generators.

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1. Introduction

A Voronoi diagram can be thought of as a map from the set of N-dimensional vectors in the domain $\Omega \subset \mathbb{R}^N$ into a finite set of vectors $\{\mathbf{z}_i\}_{i=1}^k$ called generators. It associates with each $\mathbf{z}_i$ a nearest neighbor region that is called a Voronoi region $\{V_i\}_{i=1}^k$. That is, for each i, V_i consists of all points in the domain Ω that are closer to $\mathbf{z}_i$ than to all the other generating points, and a Voronoi tessellation refers to the tessellation of a given domain into the Voronoi regions $\{V_i\}_{i=1}^k$ associated with a set of given generating points $\{\mathbf{z}_i\}_{i=1}^k \subset \Omega$ [1, 35]. With a suitably defined distortion measure, an optimal tessellation

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is given by a centroidal Voronoi tessellation, which is constructed as follows. 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

$$\mathbf{z}_i^* = \Big(\int_{V_i} \mathbf{y}\rho(\mathbf{y})\,d\mathbf{y}\Big)\Big(\int_{V_i} \rho(\mathbf{y})\,d\mathbf{y}\Big)^{-1}.$$

A *centroidal Voronoi tessellation* (CVT) is then a tessellation for which the generators of the Voronoi diagram coincide with the centroids of their respective Voronoi regions, in other words, $\mathbf{z}_i = \mathbf{z}_i^*$ for all i.

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

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

If the Voronoi tessellation $\{V_i\}_{i=1}^k$ is determined from $\{\mathbf{z}_i\}_{i=1}^k$ then we write

$$\mathscr{G}\Big(\{\mathbf{z}_i\}_{i=1}^k\Big) \equiv \mathscr{F}\Big(\{\mathbf{z}_i\}_{i=1}^k, \{V_i\}_{i=1}^k\Big). \tag{1.1}$$

The minimizer of $\mathscr{G}$ necessarily forms a CVT which illustrates the optimization property of the CVT [7]. This functional appears in many engineering applications and the relation of its minimizers with CVTs is studied, for instance, in [18, 19, 38]. For instance, it provides optimal least-squares vector quantizer design in electrical engineering applications. The CVT concept also has applications in diverse areas such as astronomy, biology, image and data analysis, resource optimization, sensor networks, geometric design, and numerical partial differential equations [2, 7–10, 12, 13, 21, 22, 25, 30, 40, 42]. In [7, 11], extensive reviews of the modern mathematical theory and diverse applications of CVTs are provided, and this list is constantly growing.

The most widely used method for computing CVTs is the algorithm developed by Lloyd in the 1960s [28]. Lloyd's algorithm represents a fixed-point type iterative algorithm consisting of the following simple steps: starting from an initial configuration (a Voronoi tessellation corresponding to an old set of generators), a new set of generators is defined by the mass centers of the Voronoi regions. The domain is re-tessellated and a new set of centroids is taken as generators. This process is continued until some stopping criterion is met. For other types of algorithms for computing CVTs we refer to [1, 11, 14, 17]. It was shown that Lloyd's algorithm decreases the energy functional $\mathscr{G}(\{\mathbf{z}_i\}_{i=1}^k)$ at every iteration, which gives strong indications of its practical convergence. Despite its simplicity, proving convergence of Lloyd's algorithm is not a trivial task. Some recent work [6, 16] has substantiated earlier claims about global convergence of Lloyd's algorithm, although single-point convergence for a general density function ρ is still not rigorously justified.

For modern applications of the CVT concept in large scale scientific and engineering problems such as data communication, vector quantization and mesh generation, it is crucial to have fast and memory-efficient algorithms for computing the CVTs. Variants of