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Estimation of Fekete points

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Abstract

We aim here at presenting a new procedure to numerically estimate the Fekete points of a wide variety of compact sets in $\mathbb{R}^3$. We understand the Fekete point problem in terms of the identification of near equilibrium configurations for a potential energy that depends on the relative position of N particles.

The compact sets for which our procedure works are basically the finite union of piecewise regular surfaces and curves. In order to determine a good initial configuration to start the search of the Fekete points of these objects, we construct a sequence of approximating regular surfaces. Our algorithm is based on the concept of disequilibrium degree, which is defined from a physical interpretation of the behavior of a system of particles when they search for a minimum energy configuration. Moreover, the algorithm is efficient and robust independently of the considered compact set as well as of the kernel used to define the energy. The numerical experimentation carried out suggests that a local minimum can be localized with a computational cost of order less than N^3.

Keywords: Fekete points; Riesz's kernels; Non-linear optimization; Potential energy; Non-smooth surfaces

1. Introduction

The problem of obtaining the Fekete points of a compact set has filled a pre-eminent place in the mathematical research during the last decades. In its original version, the problem consists in determining the position of N points of a compact subset $S \subset \mathbb{R}^2$ that maximize the product of their mutual Euclidean distances. The N-tuples, $\omega_N = \{x_1, \ldots, x_N\}$, that satisfy this property are the so-called *Nth order Fekete points* of S. It is not difficult to verify that these N-tuples minimize in S the functional

$$\mathscr{I}(\omega_N) = \sum_{1 \leqslant i < j \leqslant N} \mathscr{K}(x_i, x_j),$$

where $\mathscr{K}(x_i, x_j) = -\ln|x_i - x_j|$ is the so-called *logarithmic kernel* and $|x_i - x_j|$ is the Euclidean distance between x_i and x_j. The value $\mathscr{I}(\omega_N)$ is the *potential energy* corresponding to the logarithmic kernel when a unitary

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weight is associated with any point. In the three-dimensional Euclidean space multiple variants of the problem can be formulated by considering different kernels, among which the *Riesz's kernels*, defined as $\mathscr{K}(x_i, x_j) = |x_i - x_j|^{-s}$ with $s > 0$, constitute a family of special interest. In particular, the *Newtonian kernel*, obtained when $s = 1$, has become one of the most relevant cases and its potential energy $\mathscr{I}(\omega_N)$ is named *electrostatic potential energy*. The limit case $s \to 0$ recovers the logarithmic kernel in $\mathbb{R}^3$, whereas the case $s \to \infty$ leads to the so-called *best-packing* problem or *Tammes* problem. On the other hand, the electrostatic phenomenon in $\mathbb{R}^2$ is governed by the logarithmic kernel and the corresponding Fekete points provide "almost ideal" choices of points for polynomial interpolation [20]. Moreover, the usefulness in numerical integration of the Fekete points corresponding to the logarithmic kernel and others on the d-dimensional sphere has been showed by different authors, see for instance [5]. The logarithmic kernel also arises in the study of computational complexity. In particular, the fast generation of near optimal logarithmic energy points for the sphere in $\mathbb{R}^3$ is the focus of one of Smale's "Mathematical problems for the next century" [22]. For a more detailed description of the kernels' properties, see for instance [14].

The determination of the Fekete points of the unit sphere is considered a model of highly non-linear optimization problem with non-linear constraints. In general, only when the constraints are linear or they can be sufficiently well approximated by linear constraints it is reasonable to expect a good behavior of the usual algorithms for optimization problems with constraints. However, even in this case, the convergence ratios result lower than the ones corresponding to free optimization methods. Some authors choose to transform problems like the Fekete point one in optimization problems without constraints by considering a parametrization of the surface [16,18]. In this way, they can use classical optimization techniques such as the *Gradient* method, the *Conjugate Gradient* method, the *Newton* method and the family of *quasi-Newton* methods. Also other techniques like the so-called *Combinatory Optimization* methods have been used, among which stand out the *Simulated Annealing*, the *Tabu Search* and the *Genetic Algorithms* [16]. On the other hand, there exist few results on estimations of the Fekete points of manifolds others than the sphere. In particular, the Fekete points of the torus have been recently studied, see [9,25].

A considerable amount of theoretical and numerical results related to the different versions of the Fekete points problem have been obtained, see for instance [9–13,16,18,19,24], and it has been completely solved in some particular cases. Nevertheless, it is widely assumed that just to obtain a position near to a local optimum for hundreds of points in the sphere requires high computational resources.

In this paper, we propose an algorithm for the numerical estimation of the Fekete points of non-smooth compact sets. Essentially, these compact sets are the finite union of piecewise regular manifolds of different dimensions. We focus in the three-dimensional case, since the estimation of Fekete points is of interest in Chemistry, Biology, Nanotechnology, CAD, etc., see [1,2,9,19]. Moreover, in most of the examples we have considered the Newtonian kernel due to its special relevance, for instance in the electrical and gravitational phenomena, however we also include some examples that consider other kernels. The relation between the electrostatic potential energy of a system of particles and the energy of a distributed charge has been analyzed by several authors. In particular, the results of [12] provide us with a good framework to contrast the quality of the solutions obtained with our algorithm.

We start by describing an algorithm to estimate the Fekete points of smooth surfaces. Next, we analyze the behavior of this algorithm with the prototype problem, the unit sphere. Then, we present a transition case: we estimate the Fekete points of the unit cube by means of the algorithm for smooth surfaces, which requires the use of symmetries to reduce the domain to an open triangle. Finally, we develop a strategy for the estimation of the Fekete points of non-smooth surfaces, and we present several application examples. Throughout the paper the numerical estimation of the Fekete points of a compact set consists in identifying a local minimum from a starting configuration; *i.e.*, in obtaining a sufficiently close configuration to a local minimum in such a way that the Newton's algorithm converges.

2. Smooth surfaces

In this section, we present the fundamentals of our algorithm to estimate the Fekete points of a smooth surface. The basic structure of the algorithm is classical in the sense that each iteration consists in obtaining the advance direction and the step size in a deterministic way.