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Efficient algorithm for optimizing spectral partitions

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ABSTRACT

We present an amelioration of current known algorithms for minimizing functions depending on the eigenvalues corresponding to a partition of a given domain. The idea is to use the advantage of a representation using density functions on a fixed grid while decreasing the computational time. This is done by restricting the computation to neighbourhoods of regions where the associated densities are above a certain threshold. The algorithm extends and improves known methods in the plane and on surfaces in dimension 3. It also makes possible to make computations of optimal volumic 3D spectral partitions on sufficiently important discretizations.

1. Introduction

Many works were dedicated recently to the theoretical and numerical study of optimal spectral partitions in the plane and on surfaces in $\mathbb{R}^3$. A typical example is the minimization of the sum of the fundamental eigenvalues of the Dirichlet–Laplace operator corresponding to cells of a partition of a given domain:

$$\min_{(\omega_i)\in\mathcal{P}(D)} \lambda_1(\omega_1)+\cdots+\lambda_1(\omega_n), \tag{1}$$

where $\mathcal{P}(D)$ denotes the family of partitions into a fixed number n of cells of a domain D, belonging to $\mathbb{R}^2$, $\mathbb{R}^3$ or to a surface in $\mathbb{R}^3$. We recall that the eigenvalues of the Dirichlet–Laplace operator are obtained by solving the partial differential equation $-\Delta u=\lambda(\omega)u$ in ω with boundary condition $u=0$ on $\partial\omega$. It is known that problem (1) has a solution and the cells ω_i of the optimal partition are $C^{1,\alpha}$-regular outside singular parts of co-dimension greater than 1.

The study of spectral optimal partitioning problem (1) has multiple motivations. They are a useful tool in the proof of monotonicity formulas concerning the behaviour of solutions of PDEs on domains which are adjacent, as can be seen in [1,23]. Moreover, problem (1) appears as a limiting case in the study of chemical reactions [18] or in the study of systems of competing systems [22]. The existence of solutions for problem (1) was proved in [4] and the $C^{1,\alpha}$ regularity and qualitative properties concerning the boundaries of the cells were proved in [21,23]. The interest in numerical studies concerning problem (1) is motivated by the lack of an exact theoretical description even in the simplest cases, for small number of cells. A summary of known results for nodal and spectral partitions together with a more detailed list of references can be found in [11].

One question which remains open is the study of the spectral honeycomb problem regarding the partition of the plane which asymptotically minimizes the sum of the first eigenvalues of the Dirichlet–Laplacian of each cell. This is equivalent to studying solutions of problem (1) when $n\to\infty$. It was conjectured in [21] that the honeycomb partition is the best one. Big steps towards the proof of this conjecture were made in [9], where the authors prove that the spectral honeycomb

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conjecture is true among convex sets under the hypothesis that Polya's conjecture holds for hexagons and a slightly weaker version holds for pentagons and heptagons. We recall that Polya's conjecture states that among n-gons of fixed area, the regular one minimizes the first Dirichlet eigenvalue. Recent numerical simulations which confirm Polya's conjecture can be found in [13, Chapter 1].

The numerical aspects of the spectral partitioning problem (1) were approached by Bourdin et al. [6]. They proposed an algorithm which benefited of the fact that the cells could be represented as density functions on the same grid. This allows a straightforward implementation of a gradient based optimization method for the search of optimal numerical configurations. They managed to study partitions of up to 512 cells and they noticed that locally partitions seem to be composed of patches of regular hexagons. Due to the size of the computations the 512 cell computations was done at Texas Advanced Computing Center. Below we propose a modification of this algorithm which does not have any loss of precision and which decreases in a significant way the cost of the computation. The case of 512 cells can now be run in a reasonable amount of time on a personal computer. Some simulations for more than 1000 cells on finer discretizations are possible and some of these are presented in the following.

We recall the following works dealing with numerical computations regarding spectral optimal partitions. In [18,19] the authors present a problem issued from the modelization of chemical reactions for which the stationary state energy is the sum of the Dirichlet–Laplace eigenvalues of the cells. They present evidence that the optimal configurations approach the hexagonal one in the for large number of components. In [36], Osting et al. investigate graph partitions using spectral methods. They propose a different optimization method which is gradient free and converges to a local minimum in a finite number of iterations. In [25], the authors investigate partitions minimizing the sum of the Laplace–Beltrami eigenvalues on different surfaces in $\mathbb{R}^3$. A different approach is presented in [14] in the case of the sphere using fundamental solutions to compute the eigenvalues. An adaptation of the algorithm in [6] is presented in [17] in the case of the multiphase problem where the objective functional is the sum of the fundamental eigenvalues and an area penalization. In [15], a method for minimizing the sum of the eigenvalues and the maximal eigenvalue is proposed. In [5], the authors study the minimization of the largest eigenvalue by minimizing some p-norms of eigenvalues for large p. They propose a grid restriction procedure in the plane with the purpose of obtaining better precision. This consisted in finding rectangular neighbourhoods of the cells on which we restrict the computations. This article proposes further improvements of this procedure by considering even fewer points in the computational region. The grid restriction procedure reduces greatly the computational cost, which allows the study of partitions into a large number of cells with low computational resources. The reduction in computational complexity also allows the study of partitions on surfaces and even volumic partitions for domains in $\mathbb{R}^3$.

A similar approach was devised in [7] for the study of partitions with many cells which minimize the total perimeter. It is another example where the representation of the sets as density functions helps when dealing with partitions, which is made possible with the use of the Modica–Mortola approximations of the perimeter by Γ-convergence. For details see [8,35].

This paper focuses on describing how the methods presented in [6] can be modified so that we gain in precision and in computational speed. We underline the speed improvements which are obtained and we propose a number of simulations that can be made with this method. The method described in this article allows us to work in 3D with over one hundred cells on grids of size $100 \times 100 \times 100$. The 3D problem has also been approached in [40] for a periodic cube with a resolution of $26 \times 26 \times 26$ and up to at most three cells. In [20], the authors apply the same algorithm as in [18] to the 3D case. Recently, in [38] the authors use a diffusion generated algorithm to study optimal partitions in the periodic cube for dimension 2,3 and even 4. They also present computations regarding partitions of the sphere. The computations in [38] and [20] use an energy formulation using the diffusion equation in order to study the evolution of the partition. In [38], the use of the Fast Fourier Transform and Spherical Harmonic Transform allow to accelerate computations.

The paper is organized as follows. In Section 2, we describe the numerical algorithm for computing the eigenvalue corresponding to each cell. We also describe how to solve the eigenvalue problem on a subset of the discrete grid, which allows a great reduction in computational costs. In Section 3, we present various numerical computations showing the computational advantages of our algorithm, both in being able to efficiently solve cases where we have many cells and in solving more complex cases, like finding optimal spectral partitions of domains in $\mathbb{R}^3$. Using this algorithm we manage to give some information about the possible spectral honeycomb conjecture in $\mathbb{R}^3$. Analysing a few configurations which arise when working on the cube with periodic boundary conditions we note that the partition into rhombic dodecahedra seems to give the lowest sum of normalized eigenvalues.

2. Numerical algorithm

When considering the spectral optimal partitioning problem (1) from a numerical point of view two issues arise: first we need to be able to model the partition condition and secondly we need to be able to compute accurately enough approximations of the fundamental eigenvalues for each of the cells of the partition. In [6], both these issues were approached by replacing the cells ω_i by density functions φ_i with domain D and values in [0,1]. This immediately gives an algebraic formulation of the partition constraint, namely the sum of the functions φ_i must be identically equal to 1. The computation of the eigenvalues associated to each of the cells was made using a relaxed eigenvalue problem on the fixed domain D. The main contribution of this article is describing how the penalized eigenvalue problem can be solved in a more efficient way, by reducing the size of the computational domain around each cell.