Discrete version of an optimal partitioning problem

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Abstract

Many recent works deal with problems concerning optimal partitions related to spectral quantities of domains in Euclidean spaces or on manifolds. Due to the complexity of these problems, few explicit solutions are known. Therefore, numerical algorithms have been developed in order to find approximations of optimal partitions. Such algorithms are based on discretizations of the domain and lead to finite dimensional difference equations. In the following, the coupling of the gradient descent method with a projection algorithm leads to a non-linear difference equation. Various properties of the discrete problem are discussed and numerical results illustrating the behaviour of the discretization scheme are shown.

1 Introduction

Given an open set ω in an Euclidean space or in a manifold, the spectrum of the Laplace operator with zero Dirichlet boundary conditions consists of an increasing sequence of eigenvalues

$$0 < \lambda_1(\omega) \leq \lambda_2(\omega) \leq \cdots \to +\infty.$$

To each eigenvalue $\lambda_k(\omega)$ there corresponds an eigenfunction $u_k \in H_0^1(\omega)$ such that the following partial differential equations are satisfied:

$$\begin{cases} -\Delta u_k &= \lambda_k(\omega)u_k &\text{in } \omega \\ u_k &= 0 &\text{on } \partial\omega \end{cases}$$

Given a domain D in $\mathbb{R}^d$ or in a manifold we call a partition of D with n cells a family of sets $\omega_1, ..., \omega_n \subset D$ such that

$$\bigcup_{i=1}^{n} \omega_i = D \quad \text{and} \quad \omega_i \cap \omega_j = \emptyset.$$

The previous equalities are to be understood up to sets of zero Lebesgue measure. Optimal partition problems which are of interest in the following are related to the spectrum of the Dirichlet Laplace operator on each of the sets ω_i, $i = 1, ..., n$. We may formulate the following problems.

Problem 1. Given D in $\mathbb{R}^d$ or in a manifold, find $\omega_1, ..., \omega_n \subset D$ such that $(\omega_i)_{i=1}^n$ forms a partition of D and

$$\lambda_1(\omega_1) + \lambda_1(\omega_2) + ... + \lambda_1(\omega_n)$$

is minimized.

Problem 2. Find partitions of D such that

$$\max_{i=1,...,n} \lambda_1(\omega_i)$$

is minimized.

For simplicity, in the following we refer to Problem 1 as minimization of the sum of eigenvalues and to Problem 2 as the minimization of the max of the eigenvalues. The main point of interest of the paper is Problem 1, but similar tools can be used to study Problem 2. These problems generated a lot of interest in recent years. Since they are related to shape optimization one naturally poses the following questions:

1. Do optimal partitions exist? This was answered positively in [8] and [11].
2. What is the regularity of the boundaries of the cells? The cells have boundaries that are of class $C^{1,\alpha}$ outside singular sets of dimension $d-2$ [10],[11].
3. When are the solutions known? For Problem 1 the solutions are rarely known. For example if $n=2$ and D is a sphere then we know that two hemispheres are optimal [1]. For Problem 2 there are multiple cases which are known and techniques used are related to nodal partitions for eigenvalue problems. For more details see [5].
4. How can we approximate numerically these optimal partitions, given the bounding domain D? Due to the fact that solutions of Problems 1 and 2 are rarely known, a great interest was shown towards discretization algorithms which allow the approximation of solutions. We refer to [6], [14], [2], [15] for aspects dealing with Problem 1 and [3], [7] for Problem 2. For a more complete list of works on the subjects look at references in these cited papers.

In the following we concentrate on aspects related to Problem 1. These can be generalized to Problem 2 using techniques from [3]. Numerical methods used to approximate solutions of such spectral optimal partitioning problems use a discretization of the domain D. A method of representing the shapes which is well adapted to the study of partitions was proposed in [6] and consists of replacing each shape ω_i by a density function φ_i defined on the discrete grid. The partition condition is simply replaced by an algebraic condition on the discrete functions and can simplify the numerical treatment. It is possible to compute the derivative of the eigenvalues $\lambda_1(\omega_i)$ with respect to each of the nodes of the discretization. A gradient descent algorithm is used in order to search for a minimizer of the functional. Since performing a descent step may lead to new discrete function which may not verify the partition constraint, a projection algorithm is applied in order to make sure that the constraint is satisfied.

The above algorithm can be formulated as a non-linear recurrence relation on the discrete functions φ_i. An efficient numerical implementation is proposed, where the eigenvalue problems are solved only on a neighbourhood of the regions $\{\varphi_i \geq \varepsilon\}$ where ε is a given threshold. More details about the numerical aspects and simulation results can be found in [2]. Aspects related to the discrete algorithm are presented in the following sections, together with observations related to numerical simulations.

2 Discrete equation

In the following we present a framework for the numerical approximation of solutions of the problem

$$\min_{(\omega_i)} \lambda_1(\omega_1) + ... + \lambda_1(\omega_n), \tag{1}$$

where the minimization is made over all partitions $(\omega_i)_{i=1}^n$ of a domain D. In the applications presented below D will be a domain in the plane, in the three dimensional space or a closed surface.

In the following, for simplicity of presentation, we suppose that the domain D is the unit square. Further on we show how the general case can be handled using similar tools. Suppose that D is discretized using a $N \times N$ finite difference grid. A real function f, defined on D, is represented on the grid by its values at the $N \times N$ points: $f_{i,j}$, $1 \leq i \leq N, 1 \leq j \leq N$. We use the centred finite differences to compute the discrete Laplace operator on this grid:

$$\Delta f_{i,j} = \frac{f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1} - 4f_{i,j}}{4h^2}, \tag{2}$$

where h is the grid spacing parameter. Periodic or Dirichlet boundary conditions are used on the boundary ∂D. The discrete Laplacian is a linear operation, therefore, if we represent the values $f_{i,j}$ as a column vector $\overline{f}$ then the equation (2) can be represented as a matrix vector

product $L\overline{f}$. For simplicity, from here on, we suppose that an ordering of the $N \times N$ points is given and we label the values of the discrete function f using this labelling as f_i, $1 \le i \le N^2$. Moreover, when we drop the indices, we suppose that the operation is made on the whole vectors.

Following the results in [6], the discrete eigenvalue problem associated to a density φ_i, $1 \le i \le N^2$ defined on the finite difference grid, has the form

$$[L + C\mathrm{diag}(1 - \varphi)]u = \lambda(C, \varphi)u, \tag{3}$$

where $C \gg 1$ is a penalization parameter and $\mathrm{diag}(v)$ is a diagonal matrix with entries taken from the vector v. The results of [6] show that the derivative of the first eigenvalue of (3) with respect to the components of φ is given by

$$\partial_i \lambda_1(C, \varphi) = -Cu_i^2, \tag{4}$$

where u is a normalized eigenvector associated to $\lambda_1(C, \varphi)$ in (3).

The numerical framework presented in [6], also used in [4], [3] and [2], is based on a gradient descent algorithm, described below.

1. Given $\varphi_1, ..., \varphi_n$ densities corresponding to a partition of D (satisfying the relation $\sum_{i=1}^{n} \varphi_i = 1$), we compute the associate solutions of the discrete problem for each φ_i, given in (3).

2. The point-wise gradient with respect to each of the grid points, given in (4) can be computed.

3. We choose a step size $\alpha > 0$ and we evolve each of the densities φ_i in the opposite direction given by the gradient:
$$\varphi_i \leftarrow \varphi_i + \alpha C u_i^2 \tag{5}$$

4. The new configuration might not satisfy the partition condition. Therefore we apply a projection algorithm
$$\varphi_i \leftarrow \frac{|\varphi_i|}{\sum_{i=1}^{n} |\varphi_i|}. \tag{6}$$

This projection was proposed in [6] and has the advantage of keeping the values of the shape densities in the interval $[0, 1]$. The application $\varphi \mapsto \lambda_1(C, \varphi)$ being concave, minimizing the sum of the eigenvalues forces the values of the functions $\varphi_1, ..., \varphi_n$ towards the extreme values 0 or 1.

The composition of the transformations (5) and (6) gives the following non-linear mapping

$$(\varphi_i)_{i=1}^{n} \mapsto \frac{\varphi_i + \alpha C u_i^2}{1 + \alpha C \sum_{i=1}^{n} u_i^2}, \tag{7}$$

where u_i is the solution of (3) for $\varphi = \varphi_i$. One may note that since φ_i have values in $[0, 1]$ and the gradient descent, shown in (5), consists in adding positive quantities, the absolute values in the projection operators are no longer needed in (7).

3 Numerical results

In the following we show how the algorithm in the previous section can be implemented efficiently, in order to be able to study complex partitions from a numerical point of view. In [6] the authors used the above approach by solving the problem (3) on the whole finite-difference grid. Looking at the structure of the eigenvalue problem (3) we see that points corresponding to $\{\varphi = 0\}$ have a penalization term on the diagonal, equal to the penalization constant $C \gg 1$.
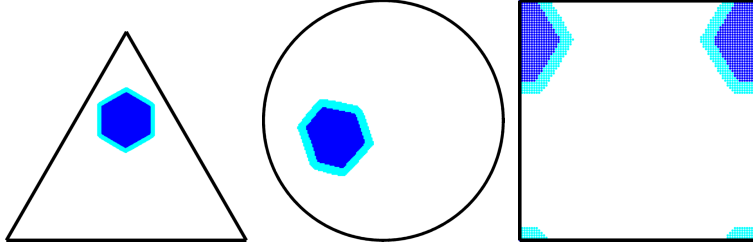
Figure 1: Reduced computational grids in various configurations.

These terms have the role of imposing the Dirichlet boundary condition. As it was noticed in [2],[3], it is not necessary to perform these computations on the whole discrete grid. Penalizing only the points which are close to the region $\{\varphi \geq \varepsilon\}$ (where ε is a chosen threshold) is enough to recover the Dirichlet boundary condition.

Therefore, using only nodes which are neighbours to the region $\{\varphi \geq \varepsilon\}$ is enough to solve the discrete eigenvalue problem (3). Moreover, using this procedure the condition number of the matrices for which we compute the eigenvalues is decreased, improving the precision of computations, and the computations are greatly accelerated since the number of nodes involved in the eigenvalue problems is reduced, especially if we have a large number of cells. In Figure 1 we show a few examples of reduced grids. The points coloured with dark blue represent points where the density φ is above 0.01. Points coloured with light blue represent neighbours of the shape, which are also included in the computation. One may observe that the size of the discrete problems is greatly reduced. In the following some applications of the improved algorithm are shown. More details can be found in [2].

In order to avoid local minima, in all computations below, the initial densities are chosen randomly and are projected onto the partition constraint. The polygonal structures in the final partitions are solely the result of the optimization algorithm.

The algorithm above was described for a finite difference grid defined on an unit square. It is possible to study general domains D by including them in a rectangular region and adding a penalization term on all nodes of the grid that are outside D.

3.1 Domains in the plane

The algorithm presented in [6] for the study of problem (1) was also capable of dealing with planar domains, but computation costs were high for many cells on fine grids. In [6] an example of computation for 512 cells on the square was presented. That computation was made on a supercomputer at the Texas Advanced Computing Center. The same computation can be done in a few hours on a laptop with the simplified algorithm using reduced grids. This result is presented in Figure 2. More complex cases can be handled, like the partition in 1000 cells on a 1000×1000 grid on the periodic square (also shown in Figure 2). It was conjectured in [10] that the partition minimizing the sum of the eigenvalues converges to the honeycomb structure as $n \to \infty$. This can be observed in Figure 2: local patches of regular hexagons appear. In order to further investigate this behaviour some computations are made on an exact union of regular hexagons. The expected behaviour is observed: the optimal partition obtained with our algorithm aligns with the exact honeycomb structure corresponding to these domains. Such a result can also be visualised in Figure 2.

Recent progress towards the proof of the spectral honeycomb conjecture was made in [9], where the authors showed that if the cells of the partitions are supposed to be convex and additional hypotheses regarding the minimality of eigenvalues of regular polygons are true, then the honeycomb partition is optimal for (1) as $n \to \infty$.
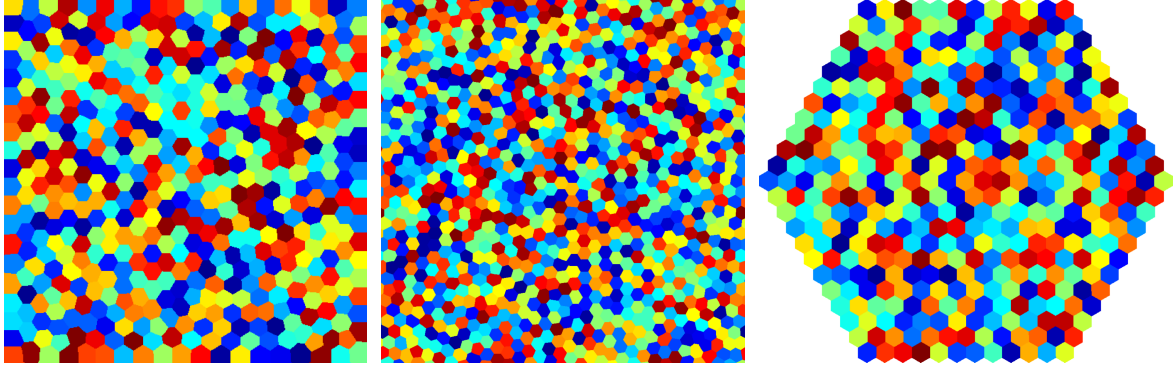
Figure 2: Optimal partitions in the plane for many cells. The cells have the tendency to distribute in a honeycomb pattern.
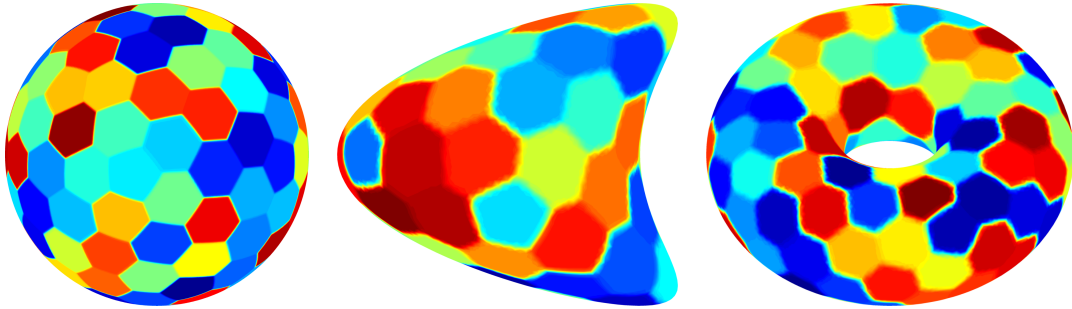

Figure 3: Partition minimizing (1) for the sphere, a torus and a more complex surface.

3.2 Domains on surfaces.

A first natural extension of the 2d algorithm is to look problem (1) for domains on surfaces in $\mathbb{R}^3$. In order to do this, a finite element setting is used to discretize the surface, but the numerical algorithm is the same. For details see [2]. In [13] the authors used an energy formulation to study optimal partitions on various surfaces. Their algorithm was also based on finite elements, using the whole triangulation for the computations. In [2] an analogue grid restriction procedure was proposed in the case of surfaces, allowing the acceleration of computations and the treatment of partitions with many cells. In this way, similar observations can be made, noting that partitions of surfaces also tend to follow the planar behaviour and patches of hexagonal cells are observed. Topological arguments based on Euler's formula show that in some cases, partitions consisting entirely of hexagons are not possible. In the case of the sphere it is observed that for n large the optimal configuration seems to consist of 12 pentagons and $n - 12$ hexagons. A few computations of optimal spectral partitions are presented in Figure 3.

3.3 Three dimensional domains

The computational simplifications due to the grid restriction procedure allow the extension of the algorithm of [6] to study problem (1) for three dimensional domains. Other works like [12] and [15] deal with three dimensional computations in periodic settings using energy formulations. The direct approach presented in the beginning of Section 2 also allows the study of non-periodic general domains. A few observations can be made in the following cases:

- **the sphere**: for $n \leq 12$ optimal partitions seem to be cones determined by subsets of the unit sphere. See Figure 4 for more details.
- **the regular tetrahedron**: for n of the form $n = k(k + 1)(k + 2)/6$ it is observed that partitions seem to be made of cells of four types corresponding to the corners, edges,

Figure 4: Partitions of the ball for $n = 4, 7, 12$. Cells of the partition are moved in order to show the interior conical structure.
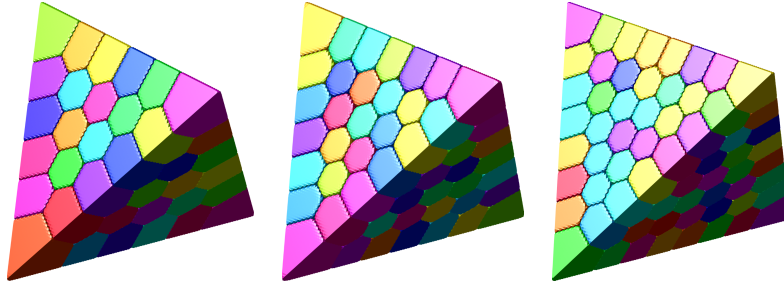

Figure 5: Partitions of the regular tetrahedron for the pyramidal numbers $n = 56, 84$ and 120.

faces and the interior of the regular tetrahedron. See Figure 5 for more details.

When n is a pyramidal number, the cells in the interior of the regular tetrahedron seem to be rhombic dodecahedra. Computations in the periodic setting for 32 cells also give the same structure. This shows important evidence toward the possible equivalent formulation of the honeycomb spectral conjecture in $\mathbb{R}^3$. A detailed analysis of the periodic case is also presented in [2].

4   Conclusions and perspectives

The algorithm of [6] was improved by considering a grid restriction procedure in order to diminish the size of the discrete eigenvalue problems. The reduction of computational time makes possible the numerical study of partitions with large number of cells for domains in $\mathbb{R}^2$, $\mathbb{R}^3$ and surfaces in $\mathbb{R}^3$. The algorithm is also an efficient tool for testing conjectures related to spectral optimal partitions.

Perspectives include the theoretical study of conjectures arising from numerical simulations. Despite the simplicity of the structures of some partitions, no progress has been made in identifying explicitly the optimal partitions solving (1). Another perspective is the study of the non-linear discrete recurrence relation (7), like showing that for α small enough the iteration provides a descent direction for (1). Finally, the convergence of the discrete algorithm could be studied by investigating the properties of the fixed point type iteration (7).

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