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A combined finite element and Bayesian optimization framework for shape optimization in spectral geometry

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This paper is dedicated to Professor Peter Monk

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A B S T R A C T

We present a novel computational framework for shape optimization problems arising in spectral geometry. The goal in such problems is to identify domains in $\mathbb{R}^d$ which are the global optima of certain functions of the spectrum of elliptic operators on the domains. We propose the use of a combined finite element and Bayesian optimization (FEM–BO) framework in this context, and demonstrate the key ideas on two concrete examples. We study the Pólya–Szegö conjecture on polygons, and demonstrate that our proposed framework yields the theoretically proven result for triangles and quadrilaterals, and also provides compelling numerical evidence for the case of pentagons. We next study a variant of this conjecture for the Steklov eigenvalue problem.

1. Introduction

In this paper we present a novel computational framework for studying shape optimization problems arising in spectral geometry. Broadly speaking, spectral geometry seeks to characterize the relationship between geometric and topological properties of a domain Ω and the spectrum of an elliptic differential operator $\mathcal{L}$ defined on Ω. We are interested specifically in isoperimetric optimization questions arising in *forward problems*: we identify an admissible class $\mathcal{A}$ of domains in $\mathbb{R}^2$ or $\mathbb{R}^3$, and seek the global optimizer $\Omega^* \in \mathcal{A}$ of a continuous function $\mathcal{F} : \mathcal{A} \to \mathbb{R}$. Here $\mathcal{F}$ is a function of the spectrum of an elliptic operator $\mathcal{L}$ on Ω.

As a prototypical instance of such problems, we recall the question asked by Lord Rayleigh in 1894: amongst all drums of a given area and tension, which one has the lowest fundamental frequency? The answer to this shape optimization question was provided by Faber [1] and Krahn [2]. They showed that the minimizer to this problem is the disk. The answers to numerous similar such optimization questions are still unknown, and are the object of intense investigation. For instance, it was shown as recently as 2015 [3] that first and third Dirichlet eigenvalues are the only eigenvalues for which the disk is the *local* minimizer amongst planar domains of fixed area. However, it is not known if the disk is the *global* minimizer of the third Dirichlet eigenvalue. (We were first made aware of this result during a seminar by A. Henrot in Banff in 2013.) Similar

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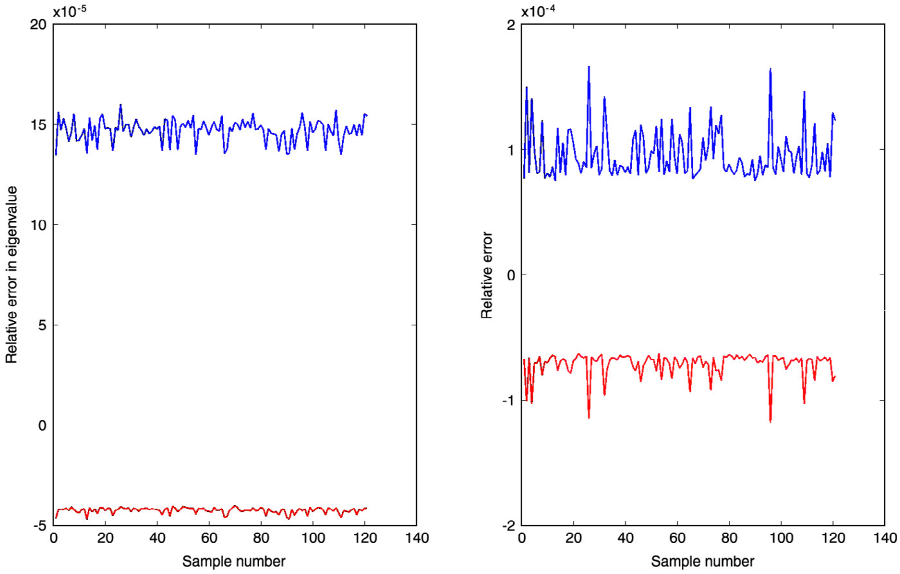

Fig. 1. The relative error in computing the first Laplace–Dirichlet eigenvalue λ_1 on rectangles of random side lengths (a, b). In red: post-processed eigenvalue bound λ_1^{nc} was computed using Crouzeix–Raviart elements. In blue: eigenvalue λ_1^{c} was computed using P1 conforming elements. Clearly $\lambda_1^{nc} \leq \lambda_1 \leq \lambda_1^{c}$ for all of the random samples. Left figure: The mesh size used for both conforming and non-conforming methods was the same. Right figure: The meshes were chosen so that the number of degrees of freedom for both the conforming and non-conforming method were within 10% of each other. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

questions may be asked for other eigenvalue problems as well. In some cases, additional properties of these eigenvalues and the admissible domains allow us, upon parametrization of the domains to constrain the search space to a compact subset of $\mathbb{R}^d$, and we are therefore guaranteed the existence of a global optimizer of $\mathcal{F}$.

Absent a mathematical argument identifying such a global optimizer, our best hope is to use careful numerical approximations. Concretely, for a given domain $\Omega \in \mathcal{A}$ we need a method to approximate the spectrum of the operator $\mathcal{L}$ and compute the objective function $\mathcal{F}(\Omega)$ and then use a method to search over $\mathcal{A}$. Both steps might require approximations, since it is only in very specific cases that $\mathcal{F}(\Omega)$ is given in closed form. In recent decades techniques from numerical analysis have been used to guide our understanding on both steps. Both the approximation of eigenvalues and the subsequent optimization can be performed in a number of ways. For example, in [4], the authors examine a variant of a level-set method for the shape optimization over a class of convex domains, and use standard finite element methods (FEM) to approximate the eigenvalues. In a different approach, Neumann eigenvalues are approximated through the method of particular solutions, and the shape optimization over the class of star-shaped domains whose boundary has a smooth (finite) Fourier representation is performed using a genetic algorithm to locate good initial guesses, and a subsequent gradient search to find the optimizer, [5]. A challenging non-smooth eigenvalue shape optimization of the ratio of the *nth* to first eigenvalue is studied using the method of particular solutions combined with a quasi-Newton (BFGS) approach in [6]. Yet another approach (for Steklov eigenvalue optimization) is proposed in [7], where the eigenvalue approximation is performed using a boundary integral approach, and the shape optimization (again over Fourier modes of the boundary curve of smooth domains) is performed using a gradient-based method.

FEM are particularly attractive for approximating eigenvalues for a variety of reasons, including provable convergence properties even in the presence of geometric or eigenfunction singularities; faithful approximation of a range of function spaces; a natural treatment of curvilinear boundaries. Additionally, there are a range of results on the use of FEM for provably bracketing of eigenvalues for a range of operators. The true eigenvalue is therefore provably between these two approximations. This is illustrated in Fig. 1 for the specific case of the eigenvalues of a simple polygon where we compare the (post-processed) eigenvalue approximations achieved by conforming and Crouzeix–Raviart finite elements. Even in situations where such bracketing results are not available, we can leverage the state-of-the-art in the area of finite element approximation of eigenvalues to obtain high-quality approximations to $\mathcal{F}(\Omega)$ for a given $\Omega \in \mathcal{A}$.

However, the question of how to optimize a general objective function $\mathcal{F}$ over $\mathcal{A}$ is more challenging. We note two important features of shape optimization problems in this context: the objective function $\mathcal{F}(\Omega)$ is an unknown, nonlinear function of the candidate domains Ω, and may have multiple local optimizers and saddles. This makes the search for global optimizers rather difficult. For example, in Fig. 2, the objective function is clearly non-convex. The shape Ω may refer to a distribution of material of different properties, and the eigenvalues can depend in a complex manner on the shape parameters. Note that in some instances, the dependence of the eigenvalue on the shape can be readily analysed. We are not advocating the use of black-box optimization strategies as a replacement for other methods in this setting, rather as a

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