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A Convex Approximation for a PDE Constrained Fractional Optimization Problem with an Application to Photonic Crystal Design

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Abstract. Based on a subspace method and a linear approximation method, a convex algorithm is designed to solve a kind of non-convex PDE constrained fractional optimization problem in this paper. This PDE constrained problem is an infinite-dimensional Hermitian eigenvalue optimization problem with non-convex and low regularity. Usually, such a continuous optimization problem can be transformed into a large-scale discrete optimization problem by using the finite element methods. We use a subspace technique to reduce the scale of discrete problem, which is really effective to deal with the large-scale problem. To overcome the difficulties caused by the low regularity and non-convexity, we creatively introduce several new artificial variables to transform the non-convex problem into a convex linear semidefinite programming. By introducing linear approximation vectors, this linear semidefinite programming can be approximated by a very simple linear relaxation problem. Moreover, we theoretically prove this approximation. Our proposed algorithm is used to optimize the photonic band gaps of two-dimensional Gallium Arsenide-based photonic crystals as an application. The results of numerical examples show the effectiveness of our proposed algorithm, while they also provide several optimized photonic crystal structures with a desired wide-band-gap. In addition, our proposed algorithm provides a technical way for solving a kind of PDE constrained fractional optimization problems with a generalized eigenvalue constraint.

AMS subject classifications: 49M37, 65K10, 90C05, 90C06, 90C26

Key words: PDE constrained optimization, fractional programming, linear approximation, finite element method, photonic band gap.

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1 Introduction

A PDE constrained optimization problem refers to the optimization of systems governed by partial differential equations (PDEs), which appear as constraints in the optimization problem [8]. In recent years, the PDE constrained optimization problem has become an important research field due to its wide application in engineering and other related fields, such as photonic crystal (PhC) structure design, liquid flow, flow control, weather forecasting, and so on [5, 6, 11, 24].

In this paper, we investigate a kind of PDE constrained optimization problem, which is in the study of the periodic band structure of micro-nanometer materials [7]. This problem can be written in the form of (1.1)

$$\begin{cases} \max\limits_{y} J(y)=\dfrac{f(y)}{g(y)} \\ \quad \text{s.t. } A(u(y))=\lambda(y)B(u(y)), \end{cases} \tag{1.1}$$

where y is the variable, and $J(y)$ is the cost functional. $f(y)$, $g(y)$, $u(y)$ and $\lambda(y)$ are functions of y. The constraint equation of (1.1) is written as a generalized eigenvalue equation, with A and B being functionals caused by the actual constraint. The problem (1.1) is an infinite-dimensional and nonlinear optimization problem with a fractional objective. These bring great difficulties to the theoretical analysis and numerical solution of this non-convex PDE constraint problem.

The photonic band gaps (PBGs) optimization problem of PhC is such a PDE constrained optimization problem in the form of the problem (1.1). As an artificial material with a periodic structure, PhCs have PBGs that can prohibit electromagnetic waves (EMWs) from propagating in certain frequency regions [2, 14, 17]. The PBGs have a wide range of industrial applications such as microwave engineering, semiconductor, laser technology, and so on [9, 10, 20, 23]. When designing PhCs, the controllable frequency bands of EMWs, i.e., the bandgap should be as big as possible to meet the actual needs. Due to the lack of fundamental length scale in Maxwell's equations, it can be shown that the magnitude of the bandgap scales by a factor of s when the crystal is expanded by a factor of $1/s$. It is more meaningful to maximize the gap ratio instead of the absolute bandgap [17]. Therefore, the objective of the PBGs optimization problem in our work is the gap ratio which is a fractional function. The propagation of electromagnetic waves can finally be governed by generalized eigenvalue equations, which is a non-convex PDE constraint of the PBGs optimization problem.

There are many approaches to solve the PBGs optimization problem, such as level set methods and other gradient-based optimization methods with prescribed inclusion shapes, fixed topology, or geometric considerations [19, 21, 29, 30]. However, gradient-based solution methods often suffer from the lack of regularity of the underlying problem when eigenvalue multiplicities are present, as they are typically at or near the solution [24, 33]. The discretization of PDE is involved when a traditional optimization