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Metamaterial filter design via surrogate optimization

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Abstract. Recently, an increasing research effort has been dedicated to analyse transmission and dispersion properties of periodic metamaterials containing resonators, and to optimize the amplitude of selected acoustic band gaps between consecutive dispersion curves in the Floquet-Bloch spectrum. Potential novel applications of this research are in the design of passive mechanical filters/diodes. The present work proposes a way to interpolate the objective functions in such band gap optimization problems, using Radial Basis Functions. The study is motivated by the high computational effort often needed for an exact evaluation of the original objective functions, when using iterative optimization algorithms. By replacing such functions with surrogate objective functions, well-performing suboptimal solutions can be obtained with a small computational effort. Numerical results demonstrate the feasibility of the approach.

1. Introduction

An increasing research effort has been recently dedicated to the analysis of transmission and dispersion properties of elastic waves propagating in periodic metamaterials containing one or more resonators per elementary cell [1,6]. These have demonstrated several improvements with respect to the associated periodic materials, which do not include the resonators. If properly designed, the geometrical and mechanical parameters of such metamaterials may allow the enhancement of specific properties. For instance, challenging issues arise in the optimization of properties of the dispersion curves for specific aims, such as opening, enlarging, closing or shifting band gaps in target acoustic frequency ranges, with potential novel applications like the design of fully customizable passive mechanical filters/diodes.

A promising approach to metamaterial design is based on formulating and solving suitable constrained nonlinear optimization problems, where the vector of optimization variables is made of design parameters such as the mass densities and radii of the resonators, the nonlinear constraints are of both mechanical and geometrical nature, and the nonlinear objective functions model any desirable property of the metamaterial, such as the amplitude of the band gap between two specific consecutive dispersion curves [2,3,4]. Unfortunately, in several cases, the application of classical iterative optimization algorithms [5] to solve such optimization problems is not easy since, at each iteration, the evaluation of the objective function can be computationally expensive (e.g., for each such evaluation, one may need to solve a sequence of eigenvalue subproblems, one for each value of the abscissa of the dispersion curves). Moreover, the associated computational effort typically increases with respect to the number of resonators per unit-cell, and to the number of design parameters to optimize [4].

By replacing the original objective functions with more-easily computable functions, surrogate optimization [10,15] can help in a first phase of the optimization, providing quickly good suboptimal solutions, to be possibly re-optimized locally in a second optimization phase, turning back to the



original objective functions. In the paper, focus is made on the application of surrogate optimization based on Gaussian Radial Basis Function (RBF) interpolation to the optimization of the filtering properties of the tetrachiral periodic metamaterial considered in the recent work [2].

The paper is organized as follows. Section 2 motivates the need for interpolation of objective functions in band gap optimization problems. Section 3 describes the solution approach adopted here, based on the combination of Gaussian RBF interpolation with an iterative optimization algorithm and a quasi-Monte Carlo multi-start technique. Section 4 reports related numerical results and discusses them.

2. Need for objective function interpolation in band gap optimization problems

Each of the constrained nonlinear optimization problems considered in [2] consists in maximizing the (normalized) amplitude of the band gap between a specific pair of consecutive dispersion curves in the acoustic part of the Floquet-Bloch spectrum. Due to space constraints, the reader is referred to [2, Section 2 and Appendix] for details about the precise physical-mathematical model, which describes a tetrachiral periodic metamaterial. Here only the following computational issues are recalled, which arise from trying to solve numerically the optimization problems above (similar issues arise for other models, e.g., the ones considered in [3,4]). For each such problem, and for any given choice of the vector of design variables, one needs the next steps to compute the associated value of the band gap:

a) determination of the coefficients of a secular equation (obtained, e.g., by evaluation of a determinant of a suitable square matrix), and computation of the (square) roots of such a secular equation. This has to be repeated for every choice of the dimensionless wave vector on the (discretized) closed boundary of the irreducible Brillouin zone, which parameterizes the square matrix itself, together with the vector of design parameters;

b) determination of maximum/minimum values of two specific consecutive dispersion curves, and their comparison.

In the above, the computational effort is dominated by step a), and increases with the dimension of the matrix involved, and with the refinement of the discretization. It is worth mentioning that a symbolic computation of the coefficients of the secular equation does not help to reduce this effort, unless the square matrix is sparse (which is usually not the case), allowing in that case a significant reduction in the number of terms appearing in the resulting symbolic expressions. Otherwise, a numeric computation of the coefficients of the secular equation for each choice of the vector of design parameters is preferable. Hence, the only way to decrease significantly the computational effort consists in reducing the number of objective function evaluations using, e.g., function interpolation.

3. Proposed solution approach

To reduce the computational effort when solving numerically each band gap optimization problem, the following surrogate optimization approach is considered in this paper. Namely, the original objective function is evaluated exactly on a finite subset of the domain to which the vector of design variables belongs (training set), then the resulting values are interpolated. Hence, the band gap optimization is performed using not the original objective function, but its interpolant. The following choices characterize the approach considered here, and distinguish it from other possible approaches based on alternative machine-learning techniques (e.g., Support Vector Machine regression [7, Section 6.2]):

a) function interpolation is used instead of function approximation, since the objective function is known exactly at the training points;

b) for the interpolation, a mesh-free method is used, based on N_c strictly positive-definite RBF computational units [8], and on a quasi-Monte Carlo discretization [11] of the domain of design variables for the selection of the centers of the RBFs (including in the training set only points generated by a quasi-Monte Carlo sequence that also satisfy all the constraints of the original optimization problem). This choice is justified by the nice approximation error guarantees (expressed in the supremum norm) available for such an interpolation scheme (see, e.g., [8, Theorem 14.5]), when the objective function is sufficiently smooth, and the fill distance (a measure of how well the training

points fill the domain) is sufficiently small. This last property is more easily obtained using a (mesh-free) quasi-Monte Carlo discretization rather than a (mesh-based) regular-grid discretization [11]. In the following, Gaussian RBFs with fixed width are used, and their common width is selected by leave-one-out cross-validation, following the approach described in [8, Section 17.1.3] and called Rippa method [12] therein. For the interpolation, the centers of the Gaussian RBFs are chosen as coincident with the training points. Hence, strict positive-definiteness of the RBFs guarantees non-singularity of the interpolation matrix, and uniqueness of the interpolant [8, Chapter 3];

c) for the optimization, a Sequential Linear Programming (SLP) algorithm including an adaptive trust region is used, employing the interpolant determined above as the surrogate objective function. This algorithm is similar to the one presented in [9] for a different application of optimization in materials science. At each iteration of the implemented algorithm, the original optimization problem is replaced by its linearization around the current vector of design variables. Changes in such variables are also limited by an additional adaptive trust region constraint, which depends on the quality of the previous linearizations. If the previous linear approximation is accurate, then the size of the trust region (which is centered on the current vector of design variables) is expanded (up to an upper bound on that size), otherwise it is reduced (up to a lower bound on it). In the paper, the SLP algorithm is applied for a fixed number N_i of iterations, although more sophisticated termination criteria may be also applied. Differently from [2,3,4], such an algorithm is used instead of the globally convergent version of the method of moving asymptotes (GCMMA) [13,14], since some preliminary simulations - whose results are not reported here, due to space constraints - have shown that, for the specific problem, the performance of the former is less dependent than the latter on the interpolation quality;

d) in a similar way as in [2,3,4], a quasi-Monte Carlo multi-start initialization approach, based on N_s different starting points for the iterative optimization algorithm, is used. In addition, a subset of the same training points used for the interpolation is selected also for the quasi-Monte Carlo multi-start initialization, since on such points there is no approximation error on the original objective function. Hence, at each initial iteration, the original objective function and the surrogate one assume the same value.

It is worth observing that the maximum value achieved by the Gaussian RBF interpolant on the whole domain does not coincide in general with the one assumed by the original objective function on the training set. For instance, when the constraints are not active at optimality, a necessary (but not sufficient) condition for having the same maximum values is that the gradient of the interpolant is equal to the all-zeros vector, for the elements of the training set associated with the maximum objective value on such a set. However, this additional condition, together with the interpolating conditions, forms a system of linear equations having typically no solution (instead, the interpolating conditions alone always determine a unique Gaussian RBF interpolant). A consequence of this is that the maximum value of the Gaussian RBF interpolant on the whole domain can be larger than the maximum value of the objective function on the training set, making the optimization of the Gaussian RBF interpolant potentially useful for the surrogate optimization of the original objective function.

4. Numerical results and discussion

In the following, numerical results are reported for the Gaussian RBF interpolant constructed as described in Section 3, by evaluating the original objective function on $N_c = 200$ centers, generated according to a Sobol' sequence [11], and satisfying all the original constraints. Then, the SLP algorithm with the adaptive trust region is applied, using the first $N_s = 10$ centers above as initial points. A variation of the optimization problem described in [2, Eq. (14)], with different bounds on the design parameters (only two of which are free), has been considered to get the numerical results presented in the following. Figure 1 illustrates, for each of the N_s repetitions of the optimization procedure above, the evolutions of the values assumed, respectively, by the surrogate and original objective functions during the iterations of the SLP algorithm (the latter values have been computed a-posteriori, for a validity check). Each repetition consists of $N_i = 100$ iterations of the SLP algorithm with the adaptive trust region. The obtained numerical results are promising since, in each repetition, the values of the

surrogate and original objective functions have evolved in a similar way (even in cases for which the quality of the interpolant may be low, possibly due to a small number of interpolation points).

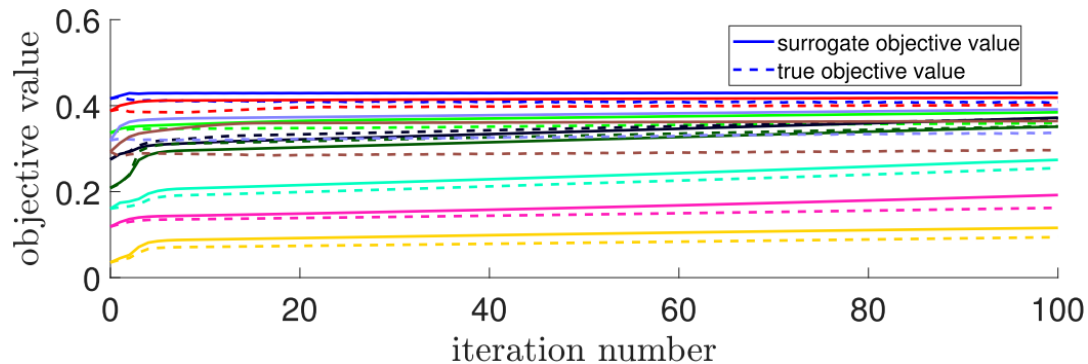


Figure 1. For each repetition of the optimization procedure: values of surrogate and original objective functions at each iteration of the SLP algorithm (same colors refer to the same repetition).

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