Inverse Scattering and Bound-Constrained Nonlinear Optimization
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Abstract

We describe an investigation into the inverse scattering problem for the Helmholtz equation in 1-d. For a fixed frequency, we attempt to find the optimal scatterer for minimizing the total transmission response given an incidental wave on the left with coefficient 1. We pose this problem as a bound-constrained optimization problem whose objective function is the norm squared of the coefficient of the transmitted wave. We briefly describe our implementation of a bound-constrained Quasi-Newton method for solving this problem in Section 3. Evaluating the objective function and its gradient requires solving the 1-d Helmholtz equation. We describe an efficient method for doing so in Section 4. The results of some numerical experiments are given in Section 5. The optimal scatterers found resemble Bragg gratings from optical fibre design.

1 Introduction

Inverse scattering problems for the Helmholtz equation are of significant interest in pure and applied mathematics [1]. The standard practice in one dimension is to consider the Helmholtz equation

\[ u_{xx} + k^2(1 + q(x))u = 0 \]

where \( q > -1 \) varies in space. We assume that \( q \) is supported on the interval \([a, b]\). We use the convention that a right-travelling wave is given by \( e^{ikx} \) and a left-travelling wave is given by \( e^{-ikx} \). For the scattering problem, we assume an incident field \( u^{(in)} = e^{ikx} \) coming from the left. Let \( u^{(sc)} \) be the scattered field, i.e., \( u = u^{(in)} + u^{(sc)} \). To specify \( u^{(sc)} \), we enforce outgoing radiation boundary conditions

\[
\left( u^{(sc)} \right)'(a) + ik u^{(sc)}(a) = 0 \quad \left( u^{(sc)} \right)'(b) - ik u^{(sc)}(b) = 0
\]

(1)

Because the incident wave is coming from the left, we know that to the right of \( b \) the function \( u \) is simply a multiple of \( e^{ikx} \). Let \( u = Te^{ikx} \) to the right of \( b \). We will refer to \( T \) as the transmission...
response to the right of $b$, a value which represents “how much” of the incident wave moves past the scatterer. Our aim is to calculate the function $q(x)$ – given a discretization of $q$ and some constraints – which will minimize the transmission response to the right of $b$.

In optical fibre design, the above is often accomplished by Bragg reflectors. These consist of alternating two different layers of material, one with a high refractive index and the other a low refractive index (for a reference, see [3]). This would correspond to a piecewise constant $q$ in the form of a square wave. The spacing and width of these layers determines which frequency is reflected the strongest and the theory applies to a long (infinite) array of these alternating layers. Our problem is posed in a similar setting; however, we are looking for the optimal $q$ over a fixed interval and our $q$ is not restricted to be one of two possible heights (it can be any height). Nonetheless, we show that the computed optimal $q$ can be quite similar in structure to a Bragg reflector.

## 2 Formulation of the Optimization Problem

To obtain a finite dimensional optimization problem, we must discretize the function $q(x)$. We choose a piecewise constant $q$ on $[a, b]$, which is equal to zero outside. We divide $[a, b]$ into $N$ uniform intervals of length $(b - a)/N$. Let $q_i$ be the value of $q$ on the $i$th interval, so that $q(x)$ is specified by the vector $\vec{q} = (q_1, \ldots, q_N)^T$. To be consistent with the design of a material, we enforce that $m \leq q(x) \leq M$ for some non-negative constants $m$ and $M$. We then define $T(\vec{q})$ to be the transmission response to the right of $b$ for the given $\vec{q}$. That is, if $u$ satisfies

$$u_{xx} + k^2(1 + q(x))u = 0$$

for an incident wave $u^{(in)} = e^{ikx}$ with the outgoing radiation conditions (1) on $u^{(sc)}$, then $T(\vec{q})$ is such that $u = T(\vec{q})e^{ikx}$ to the right of $b$. The function $T(\vec{q})$ is complex valued, so for our minimization problem, we take $|T(\vec{q})|^2$ to be our objective function. The minimization problem is then

$$\text{minimize } |T(\vec{q})|^2$$

subject to $m \leq \vec{q} \leq M$(2)

where the bounds hold component-wise for the $q_i$. This is a bound-constrained nonlinear optimization problem. We will discuss the method used for solving (2) in the next section.

## 3 Implementation of the Quasi-Newton Scheme

Because (2) has simple bound constraints, it is beneficial to use a specialized scheme rather than one which can handle general constraints. We have implemented a modified version of the scheme outlined in [2] in MATLAB. We give a brief description of this scheme here.

The bound constraints are handled by separating variables into an active set and an inactive set. The active set is defined to be those variables which are sufficiently close to their upper or lower...
bound. Restricted to these inactive variables, the search direction is chosen via a quasi-Newton method. Restricted to the active variables, the search direction is chosen to be a modified version of the steepest descent direction. In particular, if the negative gradient of an active variable points toward the active boundary, i.e. the nearby boundary, then the component for that variable is scaled so that a step of length 1 would not cause the variable to exit the feasible region.

Once the search direction is chosen, the method uses a projected search. A projected search is similar to a standard backtracking line search, with the caveat that it forces the candidate points to be in the feasible region. To determine the step length, the natural generalization of an Armijo condition to projected search is used. After each step, the approximation to the Hessian for the entire system is updated via standard BFGS.

Convergence results for this method are established in [2]. The primary assumption on the minimization problem is that the objective function is twice continuously differentiable with respect to the variables. We establish that this holds for our objective function in Section 4.

4 Evaluating the Objective Function and Gradient

Because $q$ is piecewise constant, we can come up with an analytical solution for $u$ (for a reference see [3], among others), which satisfies

$$u_{xx} + k^2(1 + q(x))u = 0$$

where $q$ is supported on the interval $[a, b]$, the incident field $u^{(in)} = e^{ikx}$, and the scattered field $u^{(sc)}$ satisfies outgoing radiation boundary conditions (1). Let $[a, b]$ be divided into $N$ subintervals with endpoints $\{a = x_1 < x_2 < \ldots < x_N < x_{N+1} = b\}$ and let $q(x) = q_l$ on $[x_l, x_{l+1}]$. The main observation is that on the interval $[x_l, x_{l+1}]$ the total field $u$ can be written as

$$u = R_le^{-ik_lx} + T_le^{ik_lx}$$

where

$$k_l = k\sqrt{1 + q_l}$$

We can then find the coefficients $R_l$ and $T_l$ by enforcing that $u$ is continuous and has continuous first derivatives across the interfaces at the $x_l$. For the interfaces at $x_1 = a$ and $x_{N+1} = b$, we note that we know the form of $u$ on $(-\infty, a)$ and $(b, \infty)$ based on our assumptions. To the left of $a$, we have

$$u = e^{ikx} + Re^{-ikx}$$

and to the right of $b$ we have

$$u = Te^{ikx}$$
due to our choice of incident field \( u^{(in)} \). Matching the function values and derivatives at the \( x_i \) gives \( 2N + 2 \) equations in the \( 2N + 2 \) unknowns \( R, T_1, R_1, \ldots, T_N, R_N, T \). The resulting system of equations has a bandwidth of five and our implementation of this routine uses the sparse matrix capabilities of MATLAB to take advantage of this structure. Once we have solved for \( v = (R, T_1, R_1, \ldots, T_N, R_N, T)^T \) it is simple to find the objective function \(|T|^2\).

To find the gradient of the objective function with respect to \( \mathbf{q} \), we note that

\[
\nabla_{\mathbf{q}} (|T|^2) = \nabla_{\mathbf{q}} (T \overline{T}) = T \nabla_{\mathbf{q}} \overline{T} + \overline{T} \nabla_{\mathbf{q}} T
\]

where \( \overline{T} \) is the complex conjugate of \( T \). So, once we’ve computed \( T \), we only need to compute \( \nabla_{\mathbf{q}} T \) to find the gradient of our objective function. If \( v \) is our vector of unknowns then

\[
Av = b
\]

where \( A \) and \( b \) enforce the continuity of \( u \) and its first derivative. The right hand side of this equation is constant in the \( q_i \). By the product rule, we have

\[
\frac{\partial A}{\partial q_i} v + A \frac{\partial v}{\partial q_i} = 0
\]  

(5)

Thus, we can find \( T_{qi} \) once we have solved for \( v \). Naively, we could use the above to compute \( v_{qi} \) for \( i = 1, \ldots, N \). This would require \( N \) backsolves of the form \( Ax = c \). We observe, however, that we are only interested in the value \( T_{qi} = e^T_N v_{qi} \), where \( e_N \) is the \( N \)th standard basis vector. We can then use the adjoint method [4] to find the \( T_{qi} \) with one backsolve. Let

\[
b_i = -\frac{\partial A}{\partial q_i} v
\]

The primary observation is that

\[
\frac{\partial T}{\partial q_i} = e^T_N \frac{\partial v}{\partial q_i} = e^T_N A^{-1} b_i = b_i^T (A^{-T} e_N)
\]

We can then find all of the \( N \) partial derivatives \( T_{qi} \) with one backsolve and \( N \) inner products, allowing for efficient computation of the gradient of \( T \) with respect to \( \mathbf{q} \). The matrix \( A_{qi} \) is extremely sparse for each \( i \) and our implementation again takes advantage of this fact when calculating \( b_i = A_{qi} v \), using the sparse matrix capacities of MATLAB.

In Section 3, we noted that our chosen optimization scheme had good convergence properties when the objective function was twice continuously differentiable. If we consider the equation (3) for \( u \) on the interval \([x_l, x_{l+1}]\) we see that the entries of \( A \) are of the form \( ce^{\pm ik_l x} \). Because the \( k_l \) are given by (4), it is then clear that \( A \) is twice continuously differentiable with respect to the \( q_l \). It then follows by differentiating (5) that \( v \) is twice continuously differentiable, and so is our objective function.
5 Numerical Experiments

We note that our problem is specified by the frequency $k$, the lower bound $m$, the upper bound $M$, the length $L$ of the interval $[a, b]$ (which we take to be $[0, L]$), and the number of subintervals $N$. We chose $L$ on the scale of a few wavelengths and $N$ so that there would be a large number of subintervals of $[0, L]$ per wavelength. We observed a few phenomena.

5.1 Square Wave Minima

For a fixed frequency, lower and upper bound, interval length, and resolution (width of the subintervals), we chose several different initial guesses $q_0$ and found that the optimizer would converge to a very similar structure for each. In the plots below, we show the initial $q_0$ in red and the result of the optimization algorithm $q$ in blue.
Despite the vastly different initial $q_0$, the optimization algorithm ended with very similar $q$. They all feature a periodic square wave, reminiscent of a Bragg grating, and most even have similar width and spacing. We number these from left to right, top to bottom. For the first, $q_0 \equiv 0$. This corresponds to a global maximum for this problem and $|T(q_0)|^2 = 1$. We actually have to add a tiny amount of noise to the computed gradient for this starting point; otherwise, the optimization wouldn’t move. The computed $q$ results in $|T(q)|^2 = 0.0129$. The second starting point $q_0$ is given as a square “bump”. The transmission coefficient for this starting point was $|T(q_0)|^2 = 0.9197$. The computed $q$ results in $|T(q)|^2 = 0.0053$. The third starting point $q_0$ is chosen at random in the feasible region. The transmission coefficient for this starting point was $|T(q_0)|^2 = 0.9807$. The computed $q$ results in $|T(q)|^2 = 0.0071$. The fourth starting point $q_0$ is a low frequency sinusoidal wave. The transmission coefficient for this starting point was $|T(q_0)|^2 = 0.9522$. The computed $q$ results in $|T(q)|^2 = 0.0045$. The fifth starting point $q_0$ is a high frequency sinusoidal wave. The transmission coefficient for this starting point was $|T(q_0)|^2 = 0.9857$. The computed $q$ results in $|T(q)|^2 = 0.0042$. The sixth starting point $q_0$ is given by $q_0 \equiv 1$. The transmission coefficient for this starting point was $|T(q_0)|^2 = 0.9201$. The computed $q$ results in $|T(q)|^2 = 0.0072$.

5.2 Fixed Number of Periods per Wavelength

For a fixed frequency, lower and upper bounds, and resolution (width of subintervals), we noticed that as you increase the length of the interval the number of square wave periods is exactly proportional to the wavelength. We ran the following experiments with random starting points and $L = 2\lambda, 4\lambda$, and $8\lambda$, where $\lambda = 2\pi/k$. (The number of periods was also consistent across frequencies). Here are the results.
For each computed $q$, there are two and a half bumps per wavelength (5, 10, and 20, respectively). Further, we noted that as the interval increased, the transmission coefficient was decreased. The computed transmission coefficients were .1191, .0052, and 1.3373e-05, respectively. This is also in congruence with the Bragg grating theory.

6 Conclusion

The numerical investigation proved interesting. We observed structures similar to Bragg gratings in our results and that these structures were consistent across the length of the interval chosen, frequency of the function, and initial guess $q_0$. In the course of solving this problem, we implemented a bound-constrained nonlinear optimization routine in MATLAB and designed and implemented an ODE solver – which could provide the gradient of the objective function – for the Helmholtz equation, also in MATLAB. More precise numerical experiments and fine tuning of the optimization routine could lead to further discoveries. Additionally, experiments could be done with different types of upper bounds (perhaps nonconstant upperbounds).
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References


