

Numerical methods for a Schrödinger equation inverse eigenvalue problem

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Abstract

We seek to solve for the potential function that satisfies the one-dimensional time-independent Schrödinger equation for a given set of eigenvalues. A variety of formulations are considered, which are all based on a discretization of this problem. The resulting systems of equations are solved using root-finding and optimization-based methods. Our results show that the success of these approaches depends on the distance between the eigenvalues.

Keywords: Quantum mechanical waves

1 Problem Setting

The Schrödinger equation plays a central role in the description of waves in quantum mechanics. It is of great practical interest to design physical systems with prescribed energy levels. Inspired by this, we consider the one-dimensional time-independent Schrödinger equation

$$-\psi_{xx}(x) + V(x)\psi(x) = \lambda\psi(x), \quad (1)$$

where $\psi(x)$, $V(x)$, and λ correspond to the wave function, potential function, and energy levels in quantum mechanics, respectively. We seek to solve for the potential function given a set of real eigenvalues. To this end, discretization of x on a grid allows the problem to be approximated as $(T + D)\vec{\psi} = \lambda\vec{\psi}$, where T is a $(-1, 2, -1)$ tridiagonal $n \times n$ matrix representing the discretized second-derivative operator and $D = \text{diag}(d_i)$ is a diagonal matrix, representing $V(x)$. Let $A = T + D$, where $a_i = 2 + d_i$ ($i = 1, \dots, n$) are the diagonal elements of A . Given a set of eigenvalues, $\vec{\lambda} = [\lambda_1 \dots \lambda_n]^T \in \mathbb{R}^n$, we seek to find $\vec{a} = [a_1 \dots a_n]^T \in \mathbb{R}^n$, such that the eigenvalues of A are $\vec{\lambda}$, that is,

$$A\vec{\psi} = \lambda\vec{\psi}, \quad (2)$$

where $\vec{\psi}$ is the corresponding eigenvector. Our objective is to develop efficient numerical approaches for solving this inverse-eigenvalue problem (IEP). IEPs come in many different forms, cf. [1], which describes both theory and numerical techniques. For several classes of IEPs, when

there are repeated eigenvalues the IEP is unsolvable almost everywhere (Theorems 3.4 and 3.10 in [1]). Hence, we require the eigenvalues to be real and distinct and assume that $\vec{\lambda}$ is ordered in increasing values.

2 System of equations formulations

There are a variety of systems of equations that can be used to solve this problem. We construct vector-valued functions for these systems of equations. The roots of these functions are solutions to (1). Formulations 1 and 2 described below are obtained using the characteristic polynomial of A . Formulation 3 involves simultaneously for $\vec{a}$ with the set of eigenvectors of A .

Formulation 1: The eigenvalues of A are the roots of its characteristic polynomial. In this study we consider the $n = 3$ case, where

$$\det(A - \lambda I_3) = -\lambda^3 + c_1(\vec{a})\lambda^2 + c_2(\vec{a})\lambda + c_3(\vec{a}), \quad (3)$$

where $c_1(\vec{a}) = a_1 + a_2 + a_3$, $c_2(\vec{a}) = -(a_1a_2 + a_1a_3 + a_2a_3 - 2)$, and $c_3(\vec{a}) = a_1a_2a_3 - (a_1 + a_3)$. As $\det(A - \lambda I) = 0$ for each $\lambda_i \in \vec{\lambda}(A)$, the requisite vector of diagonal elements, $\vec{a}$, must be a root of the vector function

$$\vec{f}_1(\vec{a}) = \begin{bmatrix} \det(A - \lambda_1 I_3) \\ \det(A - \lambda_2 I_3) \\ \det(A - \lambda_3 I_3) \end{bmatrix}.$$

More generally this would be a system of n polynomial equations of degree n for the n unknowns in $\vec{a}$.

Formulation 2: Alternatively, the characteristic polynomial can be factored as

$$\det(A - \lambda I) = (\pm 1)^{n-1}(\lambda_1 - \lambda) \dots (\lambda_n - \lambda). \quad (4)$$

Equating the coefficients in (3) and (4) yields our second vector function,

$$\vec{f}_2(\vec{a}) = \begin{bmatrix} c_1(\vec{a}) - (\lambda_1 + \lambda_2 + \lambda_3) \\ c_2(\vec{a}) - (\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3) \\ c_3(\vec{a}) - \lambda_1\lambda_2\lambda_3 \end{bmatrix}.$$

Formulation 3: Since A is symmetric, it follows that $A = P\Lambda P^T$ where $\Lambda = \text{diag}(\vec{\lambda})$ and P

is an orthogonal matrix whose columns are the eigenvectors of A . It follows that

$$AP - P\Lambda = 0 \quad \text{and} \quad PP^T = I, \quad (5)$$

Let $\vec{p} \in \mathbb{R}^{n^2}$ denote the elements of P . Using the upper triangular part of (5) yields the vector $\vec{f}_3(\vec{a}, \vec{p})$, which corresponds to $n(n+1)$ quadratic equations for the $n(n+1)$ unknowns $\vec{a}$ and $\vec{p}$.

3 Algorithms

With the goal of solving for $\vec{a}^*$ with $\vec{f}_i(\vec{a}^*) = \vec{0}$, we employ two approaches. **Method I** is a root-finding approach based on Newton's Method, which uses the Jacobian of $\vec{f}_i(\vec{a})$ for determining the iterations. **Method II** is an optimization approach that minimizes the objective function $g_i(\vec{a}) = \frac{1}{2}\|\vec{f}_i(\vec{a})\|_2^2$. Method II uses a quasi-Newton approach, which approximates the Hessian matrix using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update.

4 Initial Iterate

Root finding and optimization methods are often sensitive to the choice of initial point. To this end, the Gershgorin Circle Theorem ensures that every eigenvalue of A lies within at least one of the Gershgorin discs [2]. Applying this to the matrix A , we conclude that there exists *at least one* permutation of the eigenvalues such that if initial point $\vec{a}_0$ is equal to this permutation, then there is a "nearby" root with $\|\vec{a}^* - \vec{a}_0\|_\infty \leq 2$. As discussed below, this theorem also provides insight into the success of the numerical methods.

5 Results

To test our methods, we first generate a set of 10,000 A matrices, whose eigenvalues are real and distinct. Then, using permutations of those eigenvalues as initial points, we implemented and compared the performance of the above formulations and algorithms. These experiments show that, for all sets of eigenvalues, every combination of formulations and algorithms converge to a solution for at least one permutation of the eigenvalues as initial point. In addition, Table 1 shows the percentage of such permutations that converge to a solution for two categories of eigenvalue separation. These results show that there is a notable difference in success dependent on the minimum distance between the eigenvalues. In particular, when the eigenvalues

are well separated, i.e., if $(\Delta\lambda)_{\min} \geq 2$, where $(\Delta\lambda)_{\min} \equiv \min_{i \neq j} |\lambda_i - \lambda_j|$, the algorithms find a solution for all permutations of eigenvalues as initial points. In contrast, when $(\Delta\lambda)_{\min} < 2$, solutions are obtained for only a subset of such permutations. In addition, when $(\Delta\lambda)_{\min} < 2$ more iterations are needed to find a solution. Method I (Newton's method) finds a solution for a noticeably larger percentage of initial points than Method II (Quasi-Newton Method). For both Methods I and II, Formulations 1 and 2 perform similarly. For Method I, Formulation 3 ($\vec{f}_3(\vec{a}, \vec{p})$) finds a solution for a lower percentage of permutations, generally requires a larger number of iterates, and takes substantially more time to converge. This is likely due to the higher dimensionality of $\vec{f}_3(\vec{a}, \vec{p})$.

		$(\Delta\lambda)_{\min} < 2$	$(\Delta\lambda)_{\min} \geq 2$
Method I	$\vec{f}_1(\vec{a})$	87.63%	100.00%
	$\vec{f}_2(\vec{a})$	87.20%	100.00%
	$\vec{f}_3(\vec{a}, \vec{p})$	63.14%	100.00%
Method II	$g_1(\vec{a})$	66.97%	100.00%
	$g_2(\vec{a})$	67.05%	100.00%
	$g_3(\vec{a}, \vec{p})$	68.34%	100.00%

Table 1: Percentage of initial iterates converging to a solution using Method I (Newton's Method for finding the roots of $\vec{f}_i(\vec{a})$) and Method II (Quasi-Newton Method for minimizing $g_i(\vec{a})$). Here, $(\Delta\lambda)_{\min} \equiv \min_{i \neq j} |\lambda_i - \lambda_j|$.

6 Conclusions

We investigated numerical methods for solving an inverse eigenvalue problem associated with a 1-D time-independent Schrödinger equation. We note that all the formulations and algorithms become more sensitive to the initial point when the minimum distance between the eigenvalues is less than 2.

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