Homotopy method for the numerical solution of the eigenvalue problem of self-adjoint partial differential operators

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Given $A_1$, the discrete approximation of a linear self-adjoint partial differential operator, the smallest few eigenvalues and eigenvectors of $A_1$ are computed by the homotopy (continuation) method. The idea of the method is very simple. From some initial operator $A_0$ with known eigenvalues and eigenvectors, define the homotopy $H(t) = (1 - t)A_0 + tA_1$, $0 \leq t \leq 1$. If the eigenvectors of $H(t_0)$ are known, then they are used to determine the eigenpairs of $H(t_0 + dt)$ via the Rayleigh quotient iteration, for some value of $dt$. This is repeated until $t$ becomes 1, when the solution to the original problem is found. A fundamental problem is the selection of the step size $dt$. A simple criterion to select $dt$ is given. It is shown that the iterative solver used to find the eigenvector at each step can be stabilized by applying a low-rank perturbation to the relevant matrix. By carrying out a small part of the calculation in higher precision, it is demonstrated that eigenvectors corresponding to clustered eigenvalues can be computed to high accuracy. Some numerical results for the Schrödinger eigenvalue problem are given. This algorithm will also be used to compute the bifurcation point of a parameterized partial differential equation.

Keywords: Homotopy, eigenvalues, Rayleigh quotient iteration, Schrödinger.

1. Introduction

In this paper, we employ the homotopy method to compute the smallest few
eigenpairs (i.e., eigenvalues and their corresponding eigenvectors) of a linear self-adjoint partial differential operator. We assume that the discretization leads to a sparse matrix $A_1$ so large that standard methods, such as the QR algorithm (see Golub and Van Loan [4], for example), are not economical (or possible).

The idea of this method is rather simple. We form the homotopy:

$$H(t) = (1 - t)A_0 + tA_1, \quad 0 \leq t \leq 1,$$

where $A_0$ is some matrix whose smallest few eigenpairs are known (or can be computed relatively quickly). This is the case, for example, in numerical bifurcation problems (Keller [8]). From the known eigenpairs at time $t_0$, we obtain the eigenpairs at $t_0 + dt$ by using the Rayleigh quotient iteration (or the Rayleigh Ritz subspace iteration in case some of the eigenvalues are clustered together). Here, $dt$ is some positive number which is crucial to the efficiency of the method. Basically, $dt$ is chosen so that $H(t)$ and $H(t + dt)$ do not differ by too much. The above step is repeated until $t$ reaches 1, by that time the required eigenpairs are found.

The critical component of the Rayleigh quotient iteration is the solution of the estimate $y$ of an eigenvector,

$$(A - \lambda I)y = x,$$

where $A = H(t)$, some $t$, $\lambda$ is the current estimate of an eigenvalue, and $x$ is the old estimate of the eigenvector. Since the differential equation is self-adjoint, we assume that $A$ is a symmetric matrix. From our assumption on $A$ we must use an iterative solver rather than a direct one for this linear system. Out of convenience, we choose the preconditioned SYMMLQ iterative solver. Ruhe and Wiberg [20] have studied the case when $A$ is symmetric, positive definite. One source of difficulty is that the rate of convergence of the iterative linear solver is typically an increasing function of the condition number of the relevant matrix. This number increases as $\lambda$ approaches the actual eigenvalue. In case the actual eigenvalue is separated from the other ones, we shall see that by adding a rank-one perturbation, the resultant system

$$(A - \lambda I + xx^T)z = x$$

is better conditioned and the new solution $z$ differs from the original estimate $y$ by a scalar multiple. Here, $x$ is assumed to be normalized to length 1. This idea first appeared in Peters and Wilkinson [19] where they did not recommend its use in the context of a direct solver. However when an iterative solver is used, we find that it cuts down the number of iterations necessary for convergence.

We briefly discuss some theoretical aspects of the homotopy method applied to the matrix $A + tE$, where $A$ and $E$ are symmetric matrices. It is known (Kato [7]) that every eigenvalue $\lambda(t)$ is an analytic function of $t$ and that a corresponding orthonormal eigenvector $x(t)$ can be chosen to be an analytic function of $t$. The eigenvalue problem is

$$\left[ (A + tE)x - \lambda x \atop (1 - x^Tx)/2 \right] = 0. \quad (1)$$