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Pseudospectral methods for solving an equation of hypergeometric type with a perturbation

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ABSTRACT

Almost all, regular or singular, Sturm–Liouville eigenvalue problems in the Schrödinger form

$$-\Psi''(x) + V(x)\Psi(x) = E\Psi(x), \quad x \in (\bar{a}, \bar{b}) \subseteq \mathbb{R}, \ \Psi(x) \in L^2(\bar{a}, \bar{b})$$

for a wide class of potentials $V(x)$ may be transformed into the form

$$\sigma(\xi)y'' + \tau(\xi)y' + Q(\xi)y = -\lambda y, \quad \xi \in (a, b) \subseteq \mathbb{R}$$

by means of intelligent transformations on both dependent and independent variables, where $\sigma(\xi)$ and $\tau(\xi)$ are polynomials of degrees at most 2 and 1, respectively, and λ is a parameter. The last form is closely related to the equation of the hypergeometric type (EHT), in which $Q(\xi)$ is identically zero. It will be called here the equation of hypergeometric type with a perturbation (EHTP). The function $Q(\xi)$ may, therefore, be regarded as a perturbation. It is well known that the EHT has polynomial solutions of degree n for specific values of the parameter λ, i.e. $\lambda := \lambda_n^{(0)} = -n[\tau' + \frac{1}{2}(n-1)\sigma'']$, which form a basis for the Hilbert space $L^2(a, b)$ of square integrable functions. Pseudospectral methods based on this natural expansion basis are constructed to approximate the eigenvalues of EHTP, and hence the energies E of the original Schrödinger equation. Specimen computations are performed to support the convergence numerically.

1. Introduction

There has been a constant interest in the numerical solution of Sturm–Liouville eigenvalue problems, especially the one-dimensional Schrödinger equation described by the Hamiltonian

$$\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \quad x \in (\bar{a}, \bar{b}), \ -\infty \le \bar{a} < \bar{b} \le \infty \tag{1}$$

for a variety of quantum mechanical potentials $V(x)$. Several approximation methods have been proposed for computing the eigenvalues of the problem by numerous researchers. Among these we may recall shooting methods [1], Prüfer transformation followed by a shooting procedure [2,3], constant perturbation methods [4,5], finite difference methods [6,7], variational methods [8–10], the Wronskian approach [11], the Hill determinant method [12–14], WKB and JWKB approximations [15–20], the recursive series method [21], the path-integral approach [22] and pseudospectral methods such as the quadrature discretization method [23,24] and pseudospectral methods based on classical orthogonal polynomials [25–27].

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The so-called Liouville's transformations reduce the classical Sturm–Liouville eigenvalue problems to the Schrödinger form. In general, because of its simple structure, authors would rather approximate the Sturm–Liouville eigenvalue problems in the Schrödinger form. However, in contrast, Taşeli and Alıcı [25] transformed the Schrödinger equation over the real line

$$\mathcal{H}\Psi(x) = E\Psi(x), \quad x \in (-\infty, \infty), \ \Psi \in L^2(-\infty, \infty) \tag{2}$$

into a more complicated but beneficial form

$$y'' - 2\xi y' + \left[\xi^2 - c^{-2}V\left(c^{-1}\xi\right)\right] y = \left[1 - c^{-2}E\right] y, \quad \xi \in (-\infty, \infty) \tag{3}$$

having a regular solution $y(\xi)$ in the new independent variable ξ. Furthermore, for a symmetric potential $V(x) := v(x^2)$, they showed that another pair of special transformations lead to two similar equations

$$\xi y'' + (\gamma + 1 - \xi) y' + \frac{1}{4}\left[\xi - c^{-2}v(c^{-2}\xi)\right] y = \frac{1}{4}\left[2(\gamma + 1) - c^{-2}E\right] y, \quad \xi \in (0, \infty) \tag{4}$$

on the half-line for the treatment of even ($\gamma = -1/2$) and odd ($\gamma = 1/2$) states of (2), separately [26]. Here c appears to be a scaling parameter. One, with a closer look, can easily see that (3) and (4) resemble Hermite

$$y'' - 2\xi y' = -2ny, \quad n \in \mathbb{N} \tag{5}$$

and Laguerre

$$\xi y'' + (\gamma + 1 - \xi) y' = -ny, \quad \gamma > -1, \quad n \in \mathbb{N} \tag{6}$$

equations, respectively, especially when the modified potentials $\xi^2 - c^{-2}V\left(c^{-1}\xi\right)$ and $\frac{1}{4}\left[\xi - c^{-2}v(c^{-2}\xi)\right]$ are viewed as perturbations on the zero potential. Thus, they conclude that the Hermite basis $\{H_n(\xi)\}$ for a general potential and the Laguerre basis $\{L_n^{\gamma}(\xi)\}$ with $\gamma = \pm 1/2$ for a symmetric potential are the most appropriate choices for a pseudospectral approximation of (2).

In this article, we generalize this idea to the Schrödinger equation defined over an arbitrary subset of the real line. To this end, we consider instead of specific cases such as (5) and (6) the unperturbed case as the general EHT

$$\sigma(\xi) y'' + \tau(\xi) y' = -\lambda^{(0)} y, \quad \xi \in (a, b) \subseteq \mathbb{R} \tag{7}$$

leading not only to the Hermite and Laguerre but also the Jacobi polynomials as well. Therefore, in Section 2, we show that besides (2), certain eigenvalue problems of physical and practical interest can indeed be reduced to the form

$$\sigma(\xi) y'' + \tau(\xi) y' + Q(\xi) y = -\lambda y, \quad \xi \in (a, b) \subseteq \mathbb{R} \tag{8}$$

which we have called the EHTP. Clearly, (3) and (4) are now particular cases of (8) in this setting. In Section 3, we then construct a very general pseudospectral formulation of the EHTP based on any polynomial solutions of the EHT including every possible selection of $\sigma(\xi)$ and $\tau(\xi)$. Section 4 is concerned with the construction of a general algorithm to determine the zeros of classical orthogonal polynomials. The last section concludes the paper with numerical examples and remarks.

2. Transformation into EHTP

Excluding a few degenerate cases such as that of quadratic σ with a double root, any EHT can be transformed into a Hermite (5), Laguerre (6) or Jacobi

$$(1 - \xi^2) y'' + [\beta - \alpha - (\alpha + \beta + 2)\xi] y' = -n(n + \alpha + \beta + 1) y, \quad \alpha, \beta > -1, \ n \in \mathbb{N} \tag{9}$$

differential equation by simple scaling and shifting operations; these are called the canonical forms [28]. Accordingly, Eq. (8) with $\sigma(\xi) = 1, \xi$ and $1 - \xi^2$ will be called here the EHTP of the first, second and the third kind, respectively. Therefore, the associated unperturbed cases, that is, EHTs in (5), (6) and (9), admit the classical orthogonal polynomials as their solutions, i.e. the Hermite polynomials $H_n(\xi)$, Laguerre polynomials $L_n^{\gamma}(\xi)$ of order γ and the Jacobi polynomials $P_n^{(\alpha,\beta)}(\xi)$ of order α and β, corresponding to the three kinds of problems.

We deal with, as a first example of the second kind, the radial Schrödinger equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{M-1}{r}\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\ell(\ell + M - 2)}{r^2} + V(r)\right] \mathcal{R}(r) = E\mathcal{R}(r), \quad r \in (0, \infty), \tag{10}$$

which is naturally defined over the half-line so that $\mathcal{R}(r) \in L^2(0, \infty)$. Here, $M = 1, 2, \ldots$ and $\ell = 0, 1, \ldots$ are the space dimension and angular quantum number, respectively, and $V(r)$ is an arbitrary potential regular at the origin. Note that the Hamiltonian in (1), when considered over the half-line, is the particular case of (10) with $M = 1$ and $\ell = 0$ or $\ell = 1$. First introducing the scaled quadratic variable

$$\xi = (cr)^2, \quad c > 0, \ \xi \in (0, \infty) \tag{11}$$