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Efficient eigenvalue calculations in radiative transfer

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Abstract

An efficient method is used to compute the eigenvalues required in a discrete-ordinates solution to a special class of radiative-transfer problems. The basis for this computation is an algorithm for finding eigenvalues of a matrix that consists of the sum of a diagonal matrix and a rank-one matrix, a form that can arise in a discrete-ordinates solution of some basic transport problems. To illustrate the efficiency of the approach, a radiative-transfer problem relevant to a non-gray model with scattering that allows complete frequency redistribution is discussed.

1. Introduction

In this work, we consider a class of radiative-transfer problems based on the equation of transfer

$$\xi \frac{\partial}{\partial \tau} G(\tau, \xi) + G(\tau, \xi) = \int_{-\gamma}^{\gamma} \Psi(\xi') G(\tau, \xi') \, \mathrm{d}\xi' \tag{1}$$

for $\tau \in (0, \tau_0)$ and $\xi \in (-\gamma, \gamma)$. For the moment, in order to keep our formulation general, we do not specify the characteristic function $\Psi(\xi)$, although we do consider that $\Psi(-\xi) = \Psi(\xi)$ and that $\Psi(\xi) \geq 0$.

Commenting just briefly on the form of Eq. (1), we note, first of all, that Chandrasekhar [1] discusses "pseudo problems" that can be included in the class of problems defined by Eq. (1). In addition, McCormick and Siewert [2] and Barichello and Siewert [3], for example, have made use of various transformations to express solutions to some non-gray radiative-transfer problems with completely non-coherent scattering in terms of solutions of Eq. (1). We note too that particle-transport equations of the form of Eq. (1) are often encountered in studies in rarefied-gas dynamics [4] when a linearized form of the BGK model [5] is used.

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2. A formulation of the eigenvalue problem

In Ref. [3], especially efficient discrete-ordinates solutions to some basic problems based on Eq. (1) were formulated and evaluated numerically, and the idea of using efficient algorithms for computing the required eigenvalues, though not used, was (to the best of our knowledge) introduced into the radiative-transfer literature. The main purpose of this note is to implement this proposal. Before doing so, we review briefly the formulation of the eigenvalue problem that was reported in Ref. [3]. We start with an N-point discrete-ordinates representation of Eq. (1) written as [3]

$$\xi_i \frac{\mathrm{d}}{\mathrm{d}\tau} G(\tau, \xi_i) + G(\tau, \xi_i) = \sum_{k=1}^{N} w_k \Psi(\xi_k)[G(\tau, \xi_k) + G(\tau, -\xi_k)] \tag{2a}$$

and

$$-\xi_i \frac{\mathrm{d}}{\mathrm{d}\tau} G(\tau, -\xi_i) + G(\tau, -\xi_i) = \sum_{k=1}^{N} w_k \Psi(\xi_k)[G(\tau, \xi_k) + G(\tau, -\xi_k)] \tag{2b}$$

for $i = 1, 2, \ldots, N$. Following Ref. [3], we substitute

$$G(\tau, \pm\xi_i) = \phi(\nu, \pm\xi_i)\mathrm{e}^{-\tau/\nu} \tag{3}$$

into Eqs. (2a) and (2b) to find

$$\frac{1}{\nu}\boldsymbol{\Xi}\Phi_{+} = (\mathbf{I} - \mathbf{W})\boldsymbol{\Phi}_{+} - \mathbf{W}\boldsymbol{\Phi}_{-} \tag{4a}$$

and

$$-\frac{1}{\nu}\boldsymbol{\Xi}\boldsymbol{\Phi}_{-} = (\mathbf{I} - \mathbf{W})\boldsymbol{\Phi}_{-} - \mathbf{W}\boldsymbol{\Phi}_{+} \tag{4b}$$

where $\mathbf{I}$ is $N \times N$ identity matrix,

$$\boldsymbol{\Phi}_{\pm} = [\phi(\nu, \pm\xi_1), \phi(\nu, \pm\xi_2), \ldots, \phi(\nu, \pm\xi_N)]^{\mathrm{T}}, \tag{5}$$

$$\boldsymbol{\Xi} = \mathrm{diag}\{\xi_1, \xi_2, \ldots, \xi_N\} \tag{6}$$

and $\mathbf{W}$ is a rank-one matrix defined by the elements

$$w_{i,j} = w_j \Psi(\xi_j). \tag{7}$$

Continuing to follow Ref. [3], we let

$$\mathbf{U} = \boldsymbol{\Phi}_{+} + \boldsymbol{\Phi}_{-} \tag{8a}$$

and

$$\mathbf{V} = \boldsymbol{\Phi}_{+} - \boldsymbol{\Phi}_{-} \tag{8b}$$

so that we can eliminate **V** between the sum and the difference of Eqs. (4a) and (4b) to find

$$(\boldsymbol{\Xi}^{-2} - 2\boldsymbol{\Xi}^{-1}\mathbf{W}\boldsymbol{\Xi}^{-1})\boldsymbol{\Xi}\mathbf{U} = \frac{1}{v^2}\boldsymbol{\Xi}\mathbf{U} \tag{9}$$

where to have $\boldsymbol{\Xi}^{-1}$ exist we cannot allow any of the quadrature points $\{\xi_k\}$ to be zero. As pointed out by Barichello and Siewert [3], we can multiply Eq. (9) by a diagonal matrix **T** with the diagonal elements given, say, by

$$T_i = [w_i \Psi(\xi_i)]^{1/2} \tag{10}$$

in order to make $\mathbf{TWT}^{-1}$ symmetric; and so we can rewrite Eq. (9) as

$$(\mathbf{D} - 2\mathbf{z}\mathbf{z}^{\mathrm{T}})\mathbf{X} = \lambda\mathbf{X} \tag{11}$$

where

$$\mathbf{X} = \mathbf{T}\boldsymbol{\Xi}\mathbf{U}, \tag{12}$$

$$\mathbf{D} = \boldsymbol{\Xi}^{-2} = \mathrm{diag}\{\xi_1^{-2}, \xi_2^{-2}, \ldots, \xi_N^{-2}\}, \tag{13}$$

$$\mathbf{z} = \left[\frac{\sqrt{w_1\Psi(\xi_1)}}{\xi_1}, \frac{\sqrt{w_2\Psi(\xi_2)}}{\xi_2}, \ldots, \frac{\sqrt{w_N\Psi(\xi_N)}}{\xi_N}\right]^{\mathrm{T}} \tag{14}$$

and $\lambda = 1/v^2$. Eq. (11) establishes the eigenvalue problem we consider in this work.

3. Linear algebra

The eigenvalue problem defined by Eq. (11) has been studied extensively in the linear-algebra literature; see in particular Section 8.5.3 of Golub and Van Loan [6] and the references therein. It is known for instance that if all components of the vector **z** are non-zero, then the eigenvalues λ_i defined by Eq. (11) are simply the N zeros of the function

$$f(\lambda) = 1 - 2\mathbf{z}^{\mathrm{T}}(\mathbf{D} - \lambda\mathbf{I})^{-1}\mathbf{z}. \tag{15}$$

From the definition of **D** given by Eq. (13), it is easy to see that $f(\lambda)$ has poles at the eigenvalues of **D** (that is, $\xi_1^{-2}, \xi_2^{-2}, \ldots, \xi_N^{-2}$), and that is monotone decreasing between the poles. If the ordinates ξ_i are ordered in the usual way, we have the well-known "interlacing" result, which states that the eigenvalues λ_i are related to the diagonals of **D** in the following way:

$$\xi_1^{-2} > \lambda_1 > \xi_2^{-2} > \lambda_2 > \cdots > \xi_N^{-2} > \lambda_N.$$

If some of the components of **z** are zero, some of the strict inequalities in this expression become equalities. In particular, we have $\lambda_i = \xi_i^{-2}$ whenever $z_i = 0$.

The eigenvalues λ_i are found by identifying a root of the function $f(\lambda)$ within each of the intervals $(\xi_{i+1}^{-2}, \xi_i^{-2})$, $i = 1, 2, \ldots, N-1$, and $(-\infty, \xi_N^{-2})$. A preprocessing step handles all the zero components of $\mathbf{z}$, to yield a reduced problem in which all elements of the update vector are non-zero, and so an identification can be made between the eigenvalues λ_i and the zeros of a function of the form defined by Eq. (15). The total computation time is $O(N^2)$, since to find each of the N roots requires a modest number of evaluations of the function $f(\lambda)$ and its derivatives, where each such evaluation requires $O(N)$ arithmetic operations. This complexity compares favorably with the $O(N^3)$ complexity required for a naive application of a dense-system eigensolver to Eq. (11).

Our routines for finding the eigenvalues defined by Eq. (11) are modifications of the routines DLAED4 and DLAED8 from LAPACK [7]. The routine DLAED8 performs the preprocessing step associated with zero elements of $\mathbf{z}$. Our modification of DLAED4 finds the root of the function $f(\lambda)$ between a given pair of poles, and so it returns from each call with one of the eigenvalues λ_i. The complete set of eigenvalues λ_i, $i = 1, 2, \ldots, N$, is obtained by repeated calls of our version of DLAED4 followed by a final step to restore the eigenvalues eliminated during the preprocessing stage. Our driver routine UPDATER performs this sequence of calculations for given data $\mathbf{D}$ and $\mathbf{z}$.

We mention that the problem of finding eigenvalues of matrices that are a low-rank perturbation of matrices with known eigenvalues arises also in the context of the "divide and conquer" algorithm for tridiagonal matrices. In fact, the routines in LAPACK are geared to this particular application, which is why they require modification for our purpose.

4. Obtaining the code

Our code UPDATER, which finds the eigenvalues defined by Eq. (11) using the approach described in this work, can be obtained from the following web site:

http://www.mcs.anl.gov/~wright/dzpack/

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