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Computing the Maximal Eigenpairs of Large Size Tridiagonal Matrices with $\mathcal{O}(1)$ Number of Iterations

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Dedicated to Professor Xiaoqing Jin on the occasion of his 60th birthday

Abstract. In a series of papers, Chen [4–6] developed some efficient algorithms for computing the maximal eigenpairs for tridiagonal matrices. The key idea is to explicitly construct effective initials for the maximal eigenpairs and also to employ a self-closed iterative algorithm. In this paper, we extend Chen's algorithm to deal with large scale tridiagonal matrices with super-/sub-diagonal elements. By using appropriate scalings and by optimizing numerical complexity, we make the computational cost for each iteration to be $\mathcal{O}(N)$. Moreover, to obtain accurate approximations for the maximal eigenpairs, the total number of iterations is found to be independent of the matrix size, i.e., $\mathcal{O}(1)$ number of iterations. Consequently, the total cost for computing the maximal eigenpairs is $\mathcal{O}(N)$. The effectiveness of the proposed algorithm is demonstrated by numerical experiments.

AMS subject classifications: 60J60, 34L15

Key words: Maximal eigenpair, large size tridiagonal matrix, scaling, complexity.

1. Introduction

This paper is concerned with computing the maximal eigenpairs of tridiagonal matrices, aiming at an $\mathcal{O}(N)$ complexity for a matrix of size $N \times N$. The eigenpair here means the twins consist of eigenvalue and its eigenvector, and the maximal eigenpair indicates the largest eigenvalue and the corresponding eigenvector. The problem of computing the maximal eigenpairs has been a classical subject treated in most books of numerical analysis. The methods for this problem that are discussed most commonly are the power method, the inverse method, the Rayleigh quotient method, and some hybrid method, see, e.g., [1, 16, 17]. Finding the largest eigenpairs has many applications in signal processing, control, and recent development of Google's PageRank algorithm. On the other hand,

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numerous methods exist for the numerical computation of the eigenvalues of a real tridiagonal matrix to high accuracy. It is well known that a transformation that reduces a general matrix to Hessenberg form will reduce a Hermitian matrix to tridiagonal form. So, many eigenvalue algorithms, when applied to a Hermitian matrix, reduce the input Hermitian matrix to tridiagonal form as a first step. On the computational side, much efforts have been made to deal with symmetric tridiagonal cases, see, e.g., [2,14,15], typically requiring $\mathcal{O}(N^2)$ operations [11], although fast algorithms exist which require $\mathcal{O}(N \ln N)$ [7].

In [4], an efficient algorithm was introduced to compute the maximal eigenpair of the tridiagonal matrices with positive sub-diagonal elements. The key contribution in [4] is the explicit construction of the initial values which makes the relevant iterative algorithms unexpectedly efficient. In a following-up article [5], Chen proposed two global algorithms for computing the maximal eigenpair in a rather general setup, including a class of real (with some negative off-diagonal elements) or complex matrices.

The main idea of this work is from [5] which gives elegant formulas to approximate the largest eigenpairs in an iterative manner. It is found that for computing large scale matrices his work needs some computational polishing since possible overflows may occur when the matrix size becomes very large. The main contributions of this work is to introduce appropriate scalings to reduce the numerical instability. To make the algorithm more attractive, we also take care of the numerical complexity so that the best possible $\mathcal{O}(N)$ operations can be achieved. For nonsymmetric tridiagonal matrices, we introduce a diagonal similarity transformation to convert them into symmetric ones. Note that this symmetrization procedure can be implemented with $\mathcal{O}(N)$ operations.

One application of the fast algorithm developed in this work is to compute the largest eigenpairs of the tridiagonal random matrices. In probability theory and mathematical physics, a random matrix is a matrix-valued random variable, which in some cases share the same eigenvalues with certain tridiagonal matrices. We can take an example of the Gaussian Unitary Ensemble (GUE) which is defined as the $n \times n$ Hermitian matrices X, where the diagonal elements x_{jj} and the upper triangular elements $x_{jk} = u_{jk} + iv_{jk}$ are independent Gaussians with zero-mean. To compute the eigenpairs of X the main problem is due to the computational requirements and the memory requirements which grow fast with N. As pointed out in [9,10] computing all the eigenvalues of a full Hermitian matrix requires a computing time proportional to N^3. This means that it will take many days to create a smooth eigenvalue histogram by simulation, even for relatively small values of N, say $N = 500$. To improve upon this situation, another matrix can be studied that has the same eigenvalue distribution as X above. In [8], it was shown that this is true for the following symmetric matrix when $\beta = 2$:

$$H_\beta \sim \frac{1}{2} \begin{bmatrix} N(0,2) & \chi_{(n-1)\beta} & & & & \\ \chi_{(n-1)\beta} & N(0,2) & \chi_{(n-2)\beta} & & & \\ & \chi_{(n-2)\beta} & N(0,2) & \chi_{(n-3)\beta} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \chi_{2\beta} & N(0,2) & \chi_\beta \\ & & & & \chi_\beta & N(0,2) \end{bmatrix}.$$