Deanship of Graduate Studies

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On The Solution of Symmetric Eigenvalue Problems

By

Hammad Yousef Hammad Ealyan

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Declaration

I certify that this thesis submitted for the degree of Master is the result of my own research, except where otherwise acknowledge, and that this thesis (or any part of the same) has not been submitted for a higher degree to any other university or institution.

Signed.........................

Hammad Yousef Hammad Ealyan

Date: May 26, 2004.

Dedication

This thesis is dedicated to my parents and my family.

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Abstract

This thesis investigates a number of numerical techniques for solving symmetric eigenvalue problems. These schemes are iterative in nature, the power method and the inverse iteration are simple processes but the ideas behind them are quite far reaching. The Rayleigh quotient iteration is a version of the inverse iteration with variable shifts.

Diagonalization of symmetric matrices is employed to get other techniques such as QR method.

Newton methods are used to define new secondary linear systems of equations for the Davidson eignevalue method which leads to a new method that improves convergence.

The secondary equation avoid some common pitfalls of the Jacobi-Davidson preconditioning. We will demonstrate these schemes by some applications in various situations.

الخلاصة

الرسالة تبحث في عدد من طرق التحليل العددي لحل مسائل تتعلق بالقيم القياسية للمصفوفات المتماثلة والتي تقوم على مبدأ التكرار.

طريقة القوة وطريقة النظير من الطرق السهلة، لكن الأفكار والأساسيات التي قامت عليها ليست بالبسيطة، أما كسر ريليه فهو نسخة عن طريقة النظير مع تبديل المتغيرات. جعل المصفوفات المتماثلة محورية يساهم في طرق أخرى مثل طريقة التعامد والمثلث الأعلى، كما أن طرق نيوتن تعمل على تعريف نظام جديد من المعادلات الخطية المتعلقة بطريقة ديفيدسون والتي تؤدي إلى طريقة جديدة في إثبات التقريب، وسوف تمثل هذه الطرق بعدد من التطبيقات بأشكال مختلفة.

Contents:

Introduction

Many iterative methods for eigenvalue problems proceed almost in a similar way to solve numerically the eignvalue problem $Ax = \lambda x$. In this work, some well-known techniques are studied.

The technique developed in chapter one can be visualized as the generalization of the geometrical approach of the eigenvalue problem for 3×3 real symmetric matrices. A quadratic surface can be associated with such matrix H by means of the equation $x^T Hx = 1$ or $< Hx, x >= 1$ where $x \in R^3$. In particular, if H is a positive definite, then the corresponding surface is an ellipsoid. The vector $x_0 \in R^3$ from the origin to the farthest point in the ellipsoid can then be described as a vector at which $<x, x>$ attains the maximal value subject to the condition that x satisfies $< Hx, x >= 1$. Then, the problem can be reformulated and the side condition eliminated by asking for the minimal value of the Rayleigh quotient:

$$\frac{< Hx, x >}{< x, x >} \qquad , x \neq 0$$

the research gets underway in which centers on the remarkable fact that the number of negative pivots in the standard Gaussian elimination process applied to $A - \varepsilon I$ equals the number of A's eigenvalues less than ε.

The power method and inverse iteration are very simple processes, but the ideas behind them are quiet far reaching.

It's customary to analyze the method by means of eigenvector expansions, but a little plane trigonometry yields results which are sharper and simpler than the usual formulations.

Tridiagonal matrices have been singled out for special consideration ever since 1954 when Wallace suggested reducing matrices to this form as an intermediate stage in computing the eigenvalues of the original matrix.

The major technique for diagonalizing small tridiagonal matrices is the QR algorithm it's rather satisfying to the numerical analyst that the best method has turned out not to be some obvious technique like the power method, but a sequence of sophisticated similarity transformulation.

A parallel Davidson-type algorithm for several eigenvalues is one of many iterative methods for eigenvalue problems proceed in a similar way to obtain a solution of the eigenvalue problem $Ax = \lambda x$. They construct an orthonormal basis V and approximate the exact eigenvector x by a vector y in the subspace spanned by V. In other words, the original problem is projected onto a subspace with reduces the problem into a smaller eigenproblem $S_k y = \widetilde{\lambda} y$, where $S_k = V^T AV$.

Chapter 1

Eigenvalue Bounds

If A is a square matrix, the polynomial defined by $p(\lambda) = \det(A - \lambda I)$ is called the characteristic polynomial of A, where the root of $p(\lambda)$ are called eigenvalues of A.

If λ is an eigenvalue of A and $x \neq 0$ has the property that $(A - \lambda I)x = 0$, then x is called an eigenvector of A corresponding to the eigenvalue λ.

Useful information about the eigenvalue of A can be obtained from some of it's submatrices.

Moreover, eigenvalues of A can be related to those of neighboring matrices in a way that goes far beyond standard perturbation theory. Such investigation began in the nineteenth century and continues to this day. Much of work extends the matrix theory to cover differential and integral operators.

This chapter presents the classical matrix results and goes onto some little known refinements which have been developed in response to demands for the computation of eigenvalues of larger and ever larger matrices. All the results are inclusion theorems; that is they describe intervals which are guaranteed to contain one or more eigenvalues of A.

The later section describes stability of the numerical eigenvalue problem.

1.1. The Courant-Fisher theory

The eigenvalues of a matrix $A \in C^{n\times n}$ form a set of n points in the complex plane. Some useful ideas concerning the distribution of these points can be developed from the concept of the field of values of A, defined as the set $F(A)$ of complex numbers $\langle Ax, x\rangle$, where x ranges over all vectors in C^n that are normalized so that $\langle x, x\rangle = x^* x = 1$.

Observe that the quadratic form:

$$f(x) = \langle Ax, x\rangle = \sum_{i,j=1}^{n} a_{ij} x_i \overline{x_j}, \quad x = [x_1 \quad x_2 \quad \ldots \quad x_n]^T$$

Is a continuous function in n variables on the unit sphere in C^n, that is, the set of vectors for which $\langle x, x\rangle = \sum_{i=1}^{n} |x_i|^2 = 1$. Hence, it follows that $F(A)$ is a closed and bounded set in the complex plane. It follows also that $F(A)$ is a convex set.

Theorem 1.1.1: [8]

The field of values of the matrix $A \in C^{n\times n}$ is invariant under the unitary similarity transformation. Thus if $U \in C^{n\times n}$ is unitary, then $F(A) = F(UAU^*)$.

Proof:

We have $\langle UAU^* x, x\rangle = \langle AU^* x, U^* x\rangle = \langle Ay, y\rangle$

Where $y = U^*x$. If $\langle x, x\rangle = 1$ then $\langle y, y\rangle = \langle UU^* x, x\rangle = \langle x, x\rangle = 1$. Hence a number α is equal to $\langle UAU^* x, x\rangle$ for some $x \in C^n$ with $\langle x, x\rangle = 1$. *iff* $\alpha = \langle Ay, y\rangle$ for some normalized $y \in C^n$; that is α belongs to $F(UAU^*)$ *iff* $\alpha \in F(A)$. ■

Note that all eigenvalues of an arbitrary matrix $A \in C^{n\times n}$ are in *F(A)*. For, if $\lambda \in \sigma(A)$, then there is an eigenvector x of A corresponding to this eigenvalue for which $Ax=\lambda x$ and $\langle x, x\rangle = 1$.

Hence $\langle Ax, x\rangle = \langle \lambda x, x\rangle = \lambda\langle x, x\rangle = \lambda$, and so $\lambda \in F(A)$, thus $\sigma(A) \subset F(A)$.

Theorem 1.1.2: [8]

The field of values of a normal matrix $A \in C^{n\times n}$ coincides with the convex hull of its eigenvalues. ■

Proof:

If A is normal and it's eigenvalues are $\lambda_1, \lambda_2, ..., \lambda_n$ then there is a unitary matrix $U \in C^{n\times n}$ such that $A=UDU^*$, where $D = diag[\lambda_1, \lambda_2, ..., \lambda_n] \Rightarrow F(A) = F(D)$ where *F(D)* is the set of numbers $\alpha = \langle Dx, x\rangle = \sum_{i=1}^{n} \lambda_i |x_i|^2$ where $\langle x, x\rangle = 1$.

On the other hand, the convex hull of the points $\lambda_1, \lambda_2, ..., \lambda_n$ is the set $\left\{\sum_{i=1}^{n} \theta_i\lambda_i : \theta_i \geq 0, \sum \theta_i = 1\right\}$. Putting $\theta_i = |x_i|^2 : (i = 1,2,..., n)$ and noting that as x runs over all vectors satisfying $\langle x, x\rangle = 1$, the θ_i run over all possible choices such that $\theta_i \geq 0, \sum_{i=1}^{n} \theta_i = 1 \Rightarrow F(D)$ coincides with the convex hull of the entries on its main diagonal, we obtain the desired result. ■

For a general $n \times n$ matrix *A*, the convex hull of the points of the spectrum of a matrix *A* is a subset of *F(A)*. But for special case of the Herimitian matrices, the geometry simplifies beautifully.

Theorem 1.1.3: [8]

The field of values of the matrix $A \in C^{n\times n}$ is an interval of the real line *iff* A is Herimitian. ■

Proof:

First, if A is Herimitian then A is normal and by Theorem 1.1.2, *F(A)* is the convex hull of the eigenvalues of A, which are all real. Since the only convex sets on the real line are intervals, the required results follows.

Conversely, if $A \in C^{n\times n}$ and *F(A)* is an interval of the real line, then writing $B = \operatorname{Re} A = \frac{1}{2}(A + A^*)$, $C = \operatorname{Im} A = \frac{1}{2i}(A - A^*)$ we obtain:

$\langle Ax, x\rangle = \langle (B + iC)x, x\rangle = \langle Bx, x\rangle + i\langle Cx, x\rangle$, where $\langle Bx, x\rangle, \langle Cx, x\rangle$ are real since B and C are Hermitian. But *F(A)* consist only of real numbers, therefore $\langle Cx, x\rangle = 0$ for all x such that $\langle x, x\rangle = 1$. Hence *C=0* and *A=A**, that is A is Hermitian. ■

Corollary 1.1.4: [8]

If H is Hermetian with the eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$, then

$$F(H) = [\lambda_1, \lambda_n] \qquad (1.1.1)$$

Conversely, if $F(A) = [\lambda_1, \lambda_n]$, then A is Hermetian and λ_1, λ_n are minimal and maximal eigenvalues of A respectively. ■

Recalling the definition of *F(H)*, we deduce from Equation (1.1.1) the existence of vectors x_1, x_n on the unit sphere such that $\langle Hx_1, x_1\rangle = \lambda_1$ and $\langle Hx_n, x_n\rangle = \lambda_n$ obviously by

$$\lambda_1 = \langle Hx_1, x_1\rangle = \min_{\langle x,x\rangle=1} \langle Hx, x\rangle \qquad (1.1.2)$$