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A NEW METHOD FOR EIGENVALUE COMPUTATIONS FOR POSITIVE DEFINITE MATRICES

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ABSTRACT. In this paper, we derive and analyse a new method to compute the first few dominant eigenvalues of real positive definite matrices. It involves a variant of the power method, shifted inverse iteration and the innerproduct functional. Our method is shown to reconstruct the minimal polynomial of the matrix.

Key words and phrases: spectrum; eigenvalue; positive definite matrix.

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1. INTRODUCTION

In almost all spheres of engineering and science, knowledge of eigenvalues and eigenvectors are crucial. However, the eigenvalues λ of a $n \times n$ matrix $\mathbf{A}$ are difficult to evaluate, as the solution of the n_{th} degree characteristic equation $\det(\lambda \mathbf{I} - \mathbf{A}) = 0$ is challenging, especially for large values of n. Sometimes fairly accurate bounds for these eigenvalues will suffice. As symmetric positive definite matrices have real eigenvalues, their location is somewhat easier than the general case. In some cases only the extremal eigenvalues are required. Of particular importance are the condition number and spectral radius $\rho(\mathbf{A})$. Some crude methods of locating the spectrum are based on Gerschgorin disks and the ovals of Cassini [2]. Brauer bounds [1], using the interlacing property for Hermitian matrices and Rayleigh's quotient [7] give better results. For positive definite Toeplitz matrices Dembo [3] provided useful bounds for the extremal eigenvalues. Furthermore bounds based on traces ([11],[9],[10]) are some tools that are inexpensive, yet effective. The power method and its variants, is the classic tool to determine the extremal eigenvalues. The PageRank $PR(\mathbf{A})$ is calculated using the power method to determine the principal eigenvector of the Google matrix [6]. The power iteration is still used as in more efficient techniques like Krylov methods and the QR method. Deflation is typically used with the power method to obtain the less dominant eigenvalues. Methods by Lanczos, Arnoldi and Leverrier, amongst others, have been studied extensively to provide accurate results for $\sigma(\mathbf{A})$ [4]. Here we shall discuss a simple yet effective technique, partly based on the power method, to easily obtain the first few dominant eigenvalues. We also show that the method resembles the construction of the minimal polynomial of the matrix.

2. THEORY

Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ be a positive definite symmetric matrix, with $N \leq n$ distinct eigenvalues. Further assume that the eigenvalues $\{\lambda_i\}_{i=1}^{N}$ satisfy the descending arrangement

$$\lambda_1 > \lambda_2 > \lambda_3 \cdots > \lambda_{N-1} > \lambda_N. \tag{2.1}$$

Remark 2.1. The corresponding orthonormal eigenbasis of $\mathbf{A}$ is given by

$$S = \{\mathbf{u}_i^j \,| i = 1,\, 2, \cdots, N; j = 1,\, 2, \cdots, m_i\}. \tag{2.2}$$

We shall refer to λ_i as **dominant** to λ_j, whenever $\lambda_i > \lambda_j$. Let $f(z)$ be a positive increasing function defined on the spectrum $\sigma(\mathbf{A})$, such that $f(\mathbf{A})$ is symmetric. Thus $f(\lambda_{i+1}) > f(\lambda_i), i = 1, 2, \cdots, N-1$. Let $\mathbf{x}_0 \in \mathbb{R}^n$ be randomly chosen so that $\|\mathbf{x}_0\|_2 = 1$, then by the spectral theorem for diagonalizable matrices [8] we have that

$$\mathbf{x}_0 = \sum_{j=1}^{N} \mathbf{G}_j \mathbf{x}_0, \tag{2.3}$$

where $\mathbf{G}_j$ is the projector onto the null space $N(\mathbf{A} - \lambda_j \mathbf{I})$. Recall that $\mathbf{G}_i\mathbf{G}_j = \delta_{ij}\mathbf{G}_i$, where δ_{ij} denotes the Kronecker delta symbol. We have also that

$$\begin{aligned} f(\mathbf{A}) &= \sum_{i=1}^{N} f(\lambda_i)\mathbf{G}_i \\ &= \sum_{i=1}^{N} f_i \mathbf{G}_i, \end{aligned} \tag{2.4}$$

where we have introduced the notation $f_i = f(\lambda_i)$ for brevity. Thus

$$f(\mathbf{A})\mathbf{x}_0 = \sum_{i=1}^{N} f_i \mathbf{G}_i \mathbf{x}_0 \tag{2.5}$$

$$f(\mathbf{A})^k\mathbf{x}_0 = \sum_{i=1}^{N} f_i^k \mathbf{G}_i \mathbf{x}_0. \tag{2.6}$$

Let $d_k = \langle f(\mathbf{A})^k\mathbf{x}_0, \mathbf{x}_0\rangle$, then

$$\begin{aligned} d_k &= \left\langle \sum_{i=1}^{N} f_i^k \mathbf{G}_i \mathbf{x}_0, \sum_{i=1}^{N} \mathbf{G}_j \mathbf{x}_0 \right\rangle \\ &= \sum_{i=1}^{N} \|\mathbf{G}_i\mathbf{x}_0\|_2^2 f_i^k \\ &= \sum_{i=1}^{N} c_i^2 f_i^k \\ &= \sum_{i=1}^{p} c_i^2 f_i^k + \sum_{i=p+1}^{N} c_i^2 f_i^k, \end{aligned} \tag{2.7}$$

where $c_i = \pm\|\mathbf{G}_i\mathbf{x}_0\|_2$. From (2.7) we may write

$$d_{k+j} = \sum_{i=1}^{p} c_i^2 f_i^{k+j} + \sum_{i=p+1}^{N} c_i^2 f_i^{k+j}, \tag{2.8}$$

$j = 0, 1, \ldots, 2p-1$.
For suitable k large enough in (2.8), we may ignore the second expression, as $|c_i| \leq 1$, $f_p^k >> f_{p+1}^k$, and the contribution due to the latter is negligible in finite digit arithmetic. We thus write

$$d_{k+j} = \sum_{i=1}^{p} c_i^2 f_i^{k+j},\ j = 0, 1, \cdots, 2p-1. \tag{2.9}$$

The latter represents a system of $2p$ non-linear equations in $2p$ unknowns $c_i, \lambda_i,\ i = 1, 2, \cdots, p$. For $p = 1$ in (2.9) we have

$$d_k = c_1^2 f_1^k \tag{2.10}$$

$$d_{k+1} = c_1^2 f_1^{k+1}, \tag{2.11}$$

so that

$$f_1 = \frac{d_{k+1}}{d_k}. \tag{2.12}$$

Thus for $p = 1$ we get (2.12) which is equivalent to the power method. For $p = 2$ in (2.9) we get

$$d_k = c_1^2 f_1^k + c_2^2 f_2^k \tag{2.13}$$

$$d_{k+1} = c_1^2 f_1^{k+1} + c_2^2 f_2^{k+1} \tag{2.14}$$

$$d_{k+2} = c_1^2 f_1^{k+2} + c_2^2 f_2^{k+2} \tag{2.15}$$

$$d_{k+3} = c_1^2 f_1^{k+3} + c_2^2 f_2^{k+3}. \tag{2.16}$$

Equation (2.13) is multiplied by f_1 and (2.14) is subtracted from (2.13). A similar process is applied to the remaining equations to yield

$$f_1 d_k - d_{k+1} = c_2^2 f_2^k (f_1 - f_2) \tag{2.17}$$

$$f_1 d_{k+1} - d_{k+2} = c_2^2 f_2^{k+1} (f_1 - f_2) \tag{2.18}$$

$$f_1 d_{k+2} - d_{k+3} = c_2^2 f_2^{k+2} (f_1 - f_2). \tag{2.19}$$

Equation (2.18) is divided by equation (2.17) and equation (2.19) is divided by (2.18) to yield

$$\begin{aligned} f_2 &= \frac{f_1 d_{k+1} - d_{k+2}}{f_1 d_k - d_{k+1}} \\ &= \frac{f_1 d_{k+2} - d_{k+3}}{f_1 d_{k+1} - d_{k+2}} \end{aligned} \tag{2.20}$$

From (2.20) we deduce that f_1 satisfies the quadratic equation

$$a f_1^2 + b f_1 + c = 0, \tag{2.21}$$

where $a = d_{k+1}^2 - d_k d_{k+2}$,
$b = d_k d_{k+3} - d_{k+1} d_{k+2}$, and $c = d_{k+2}^2 - d_{k+1} d_{k+3}$.

Theorem 2.1. *The quadratic equation* (2.21) *has two positive roots.*

Proof:
From equations (2.13)-(2.15) we have that

$$\begin{aligned} a &= d_{k+1}^2 - d_k d_{k+2} \\ &= c_1^4 f_1^{2k+2} + c_2^4 f_2^{2k+2} + 2c_1^2 c_2^2 f_1^{k+1} f_2^{k+1} \\ &- c_1^4 f_1^{2k+2} - c_2^4 f_2^{2k+2} - c_1^2 c_2^2 f_1^k f_2^{k+2} \\ &- c_1^2 c_2^2 f_1^{k+2} f_2^k \\ &= c_1^2 c_2^2 f_1^k f_2^k (2 f_1 f_2 - f_1^2 - f_2^2) \\ &= -c_1^2 c_2^2 f_1^k f_2^k (f_1 - f_2)^2 \end{aligned} \tag{2.22}$$

Similarly we may show that

$$b = c_1^2 c_2^2 f_1^k f_2^k (f_1 - f_2)^2 (f_1 + f_2) \tag{2.23}$$

$$c = -c_1^2 c_2^2 f_1^{k+1} f_2^{k+1} (f_1 - f_2)^2. \tag{2.24}$$

Thus the discriminant can be shown to be

$$b^2 - 4ac = c_1^4 c_2^4 f_1^{2k} f_2^{2k} (f_1 - f_2)^6 > 0. \tag{2.25}$$

Thus complex roots are excluded. Since f_1 is one root and the sum of the roots is $\frac{-b}{a} = f_1 + f_2$, it follows that f_2 is the smaller root that also satisfies (2.21). For $p = 3$ in (2.9) we get a non-linear system of six unknowns in six equations. It is however challenging and not necessary to solve this system. Having obtained f_1 and f_2, we solve just the first four equations namely:

$$d_k = c_1^2 f_1^k + c_2^2 f_2^k + c_3^2 f_3^k \tag{2.26}$$

$$d_{k+1} = c_1^2 f_1^{k+1} + c_2^2 f_2^{k+1} + c_3^2 f_3^{k+1} \tag{2.27}$$

$$d_{k+2} = c_1^2 f_1^{k+2} + c_2^2 f_2^{k+2} + c_3^2 f_3^{k+2} \tag{2.28}$$

$$d_{k+3} = c_1^2 f_1^{k+3} + c_2^2 f_2^{k+3} + c_3^2 f_3^{k+3}, \tag{2.29}$$

for f_3. Notice that

$$\begin{aligned} & d_{k+2} - (f_1 + f_2)d_{k+1} + f_1 f_2 d_k \\ & = c_3^2 f_3^k (f_3 - f_1)(f_3 - f_2) \end{aligned} \tag{2.30}$$

$$\begin{aligned} & d_{k+3} - (f_1 + f_2)d_{k+2} + f_1 f_2 d_{k+1} \\ & = c_3^2 f_3^{k+1} (f_3 - f_1)(f_3 - f_2) \end{aligned} \tag{2.31}$$

Thus f_3 is obtained from the ratio

$$f_3 = \frac{d_{k+3} - (f_1 + f_2)d_{k+2} + f_1 f_2 d_{k+1}}{d_{k+2} - (f_1 + f_2)d_{k+1} + f_1 f_2 d_k} \tag{2.32}$$

Having found $f_1,\ f_2,\ f_3, \cdots, f_{q-1}$, a similar procedure of deriving f_3 is applied to derive the following expression for f_q, namely

$$f_q = \frac{\sum_{j=0}^{q-1} (-1)^j S_j d_{k+q-j}}{\sum_{j=0}^{q-1} (-1)^j S_j d_{k+q-j-1}} \quad q \geq 3. \tag{2.33}$$

Here

$$S_j = \sum_{1 \leq i_1 < \cdots < i_j \leq q-1} f_{i_1} \cdots f_{i_j} \tag{2.34}$$

is the symmetric sum of $f_1,\ f_2, \cdots f_{q-1}$, that is the sum of the product of all f_i taken j at a time.

Theorem 2.2. *The process advocated by equation* (2.32) *is unstable unless f_1 and f_2 are fairly accurate.*

Proof:
Let ϵ_1 and ϵ_2 be perturbations of f_1 and f_2 respectively and write $\hat{f}_1 = f_1 + \epsilon_1$ and $\hat{f}_2 = f_2 + \epsilon_2$, then from (2.32) we obtain

$$\hat{f}_3 = \frac{d_{k+3} - (\hat{f}_1 + \hat{f}_2)d_{k+2} + \hat{f}_1 \hat{f}_2 d_{k+1}}{d_{k+2} - (\hat{f}_1 + \hat{f}_2)d_{k+1} + \hat{f}_1 \hat{f}_2 d_k} \tag{2.35}$$

$$\begin{aligned} &= \frac{\begin{pmatrix} d_{k+3} - (f_1 + f_2 + \epsilon_1 + \epsilon_2)d_{k+2} \\ +(f_1 + \epsilon_1)(f_2 + \epsilon_2)d_{k+1} \end{pmatrix}}{\begin{pmatrix} d_{k+2} - (f_1 + f_2 + \epsilon_1 + \epsilon_2)d_{k+1} \\ +(f_1 + \epsilon_1)(f_2 + \epsilon_2)d_k \end{pmatrix}} \\ &= \frac{N - (\epsilon_1 + \epsilon_2)d_{k+2} + (f_1\epsilon_2 + f_2\epsilon_1)d_{k+1}}{D - (\epsilon_1 + \epsilon_2)d_{k+1} + (f_1\epsilon_2 + f_2\epsilon_1)d_k}, \end{aligned} \tag{2.36}$$

where we have retained first order perturbations and $N = d_{k+3} - (f_1 + f_2)d_{k+2} + f_1 f_2 d_{k+1}$, $D = d_{k+2} - (f_1 + f_2)d_{k+1} + f_1 f_2 d_k$ are the numerator and denonimator of (2.32) respectively. Thus

$$\begin{aligned} \hat{f}_3 &= \frac{N}{D} \left(1 - \frac{(\epsilon_1 + \epsilon_2)d_{k+2} + (f_1\epsilon_2 + f_2\epsilon_1)d_{k+1}}{N}\right) \\ &\quad \left(1 - \frac{(\epsilon_1 + \epsilon_2)d_{k+1} + (f_1\epsilon_2 + f_2\epsilon_1)d_k}{D}\right)^{-1} \\ &= f_3 \left(1 - \frac{(\epsilon_1 + \epsilon_2)d_{k+2} + (f_1\epsilon_2 + f_2\epsilon_1)d_{k+1}}{N}\right) \\ &\quad \left(1 + \frac{(\epsilon_1 + \epsilon_2)d_{k+1} + (f_1\epsilon_2 + f_2\epsilon_1)d_k}{D} + \cdots\right). \end{aligned} \tag{2.37}$$

Therefore to first order perturbations

$$\epsilon_3 = \hat{f}_3 - f_3$$

$$= f_3 \left(\frac{(\epsilon_1 + \epsilon_2)d_{k+1} + (f_1\epsilon_2 + f_2\epsilon_1)d_k}{D} - \tag{2.38}\right.$$

$$\left. \frac{(\epsilon_1 + \epsilon_2)d_{k+2} + (f_1\epsilon_2 + f_2\epsilon_1)d_{k+1}}{N} \right) \tag{2.39}$$

We thus see that ϵ_3 depends on the products $f_3 f_1 \epsilon_2$ and $f_3 f_2 \epsilon_1$. If f_1 or f_2 are not fairly accurate, namely ϵ_1 and ϵ_2 are not very small, then the two products can be significant depending on how large $f_3 f_1$ and $f_3 f_2$ are. This will result in an inaccurate calculated value for f_3.

Lemma 2.3. *The solution of the difference equation from* (2.33) *is intimately related to the minimal polynomial of* $f(\mathbf{A})$.

Proof:
Rewrite equation (2.33) as

$$f_q \sum_{j=0}^{q-1} (-1)^j S_j d_{k+q-j-1} = \sum_{j=0}^{q-1} (-1)^j S_j d_{k+q-j} \quad q \geq 3. \tag{2.40}$$

Let $d_r = \lambda^r$ in (2.40) and simplify to get

$$f_q \sum_{j=0}^{q-1} (-1)^j S_j \lambda^{q-j-1} = \sum_{j=0}^{q-1} (-1)^j S_j \lambda^{q-j} \quad q \geq 3, \tag{2.41}$$

and hence

$$(\lambda - f_q) \sum_{j=0}^{q-1} (-1)^j S_j \lambda^{q-j-1} = 0. \tag{2.42}$$

The left hand side of equation (2.42) is equivalent to the first q linear factors of the minimal polynomial of $f(\mathbf{A})$, namely.

$$(\lambda - f_q)(\lambda - f_{q-1}) \cdots (\lambda - f_1). \tag{2.43}$$

The following algorithm is advocated to calculate the first say $f_i, \ i = 1, 2, 3, 4$.

Algorithm 1

choose $\mathbf{x}_0 \in \mathbb{R}^n$ randomly, $\|\mathbf{x}_0\|_2 = 1$,
and an appropriate tolerance ε_1.
for $k = 1$ to K (some max number of iterations)
$\mathbf{x}_k = \mathbf{A}\mathbf{x}_{k-1}$
$\mathbf{x}_k = \dfrac{\mathbf{x}_k}{\|\mathbf{x}_k\|_2}$ (a)
store $\mathbf{x}_k$
$\mathbf{err} = \|\mathbf{x}_k - \mathbf{x}_{k-1}\|_2$
if $\mathbf{err} \le \varepsilon_1; k = k_1;$ **break**; **end if**
$\mathbf{x}_{k-1} = \mathbf{x}_k$
end for statement
set $k = k_1, \ \ d_k = \langle \mathbf{x}_k, \mathbf{x}_0 \rangle;$
$d_{k+1} = \langle \mathbf{A}\mathbf{x}_k, \mathbf{x}_0 \rangle; d_{k+2} = \langle\ \mathbf{A}(\mathbf{A}\mathbf{x}_k), \mathbf{x}_0 \rangle$ (b)
solve the quadratic (2.21) for f_1 and f_2
use the shifted inverse power method on ($\mathbf{A} - f_1\mathbf{I}$) (c)
with two iterations to obtain f_1 accurately
repeat step (c) for f_2
repeat step (b) with k replaced by $\lfloor \frac{k_1}{2} \rfloor$
to calculate up to d_{k+3}
Use (2.32) **to evaluate** f_3
repeat step (c) for f_3
repeat step (b) with k replaced by $\lfloor \frac{k_1}{4} \rfloor$
to calculate up to d_{k+4}
use (2.33) **to evaluate** f_4
repeat step (c) for f_4

It is necessary to scale the iterates in step (a) to prevent numerical overflow. Scaling does not affect our derivation of f_i. Step (c) is necessary to accurately determine f_i before proceeding to the calculation of f_{i+1} as shown in Theorem 1. In addition it also yields the corresponding eigenvector. In all our examples we use $f(x) = x$ for convenience. It is possible to use $f(x) = x^2$ especially when the separation of λ_1 and λ_2 is very small, to avoid using a large value for k (which corresponds to more iterations).

Example 2.1. *Consider the matrix* [5]

$$\begin{bmatrix} 5 & 7 & 6 & 5 \\ 7 & 10 & 8 & 7 \\ 6 & 8 & 10 & 9 \\ 5 & 7 & 9 & 10 \end{bmatrix}$$

with distinct eigenvalues. Let $\hat{\sigma}(\mathbf{A})$ denote the calculated spectrum according to our algorithm. Both the exact and approximate spectrums are displayed in table 2.1 accurate to sixteen significant digits.

Table 2.1: Spectrum: example 1

$\sigma(\mathbf{A})$	$\hat{\sigma}(\mathbf{A})$
0.01015004839789208	0.01015004839789159
0.84310714985503320	0.84310714985503290
3.85805745594494900	3.85805745594495080
30.28868534580212000	30.28868534580212600

Here the errors are $\mathcal{O}(10^{-15})$.

Example 2.2. *Consider the matrix* [5]

$$\begin{bmatrix} 8 & 4 & 4 & 1 \\ 4 & 8 & 1 & 4 \\ 4 & 1 & 8 & 4 \\ 1 & 4 & 4 & 8 \end{bmatrix}$$

with $\sigma(\mathbf{A}) = \{1\,, 7\,, 7\,, 17\}$. Our algorithm is able to produce $\tilde{\sigma}(\mathbf{A}) = \{1\,, 7\,, 17\}$, consistent with our theory that cannot detect repeated eigenvalues.

Example 2.3. *Consider the tridiagonal matrix* [5]*,*

$$\begin{bmatrix} 2 & 2 & 1 & 0 & 0 & 0 \\ 2 & 3 & 2 & 1 & 0 & 0 \\ 1 & 2 & 3 & 2 & 1 & 0 \\ 0 & 1 & 2 & 3 & 2 & 1 \\ 0 & 0 & 1 & 2 & 3 & 2 \\ 0 & 0 & 0 & 1 & 2 & 2 \end{bmatrix},$$

where the eigenvalues are given by $\lambda_i = 4\cos(\frac{i\pi}{7})(\cos(\frac{i\pi}{7}) - 1) + 1,\ i = 1, 2, \ldots, 6$

Table 2.2: Spectrum:example 3

$\sigma(\mathbf{A})$	$\hat{\sigma}(\mathbf{A})$
0.06099892465243698	0.06099892465243717
0.30797852836990410	0.30797852836990390
0.64310413210779050	0.64310413210779040
2.08814600002041750	2.08814600002041930
5.04891733952230750	5.04891733952230500
7.85085507532714300	7.85085507532714400

Here we had to use 4 shifted inverse iterations to acquire the first two entries in table 2.2 to $\mathcal{O}(10^{-15})$.

3. CONCLUSION

We have derived and presented a new innovative algorithm to calculate the eigenvalues of symmetric positive definite matrices. We note that it is a useful procedure to calculate the first few dominant eigenvalues. This is attributed to the extra number of shifted inverse iterations required for proceeding further. In addition our method does not require deflation, though it does provide the corresponding eigenvectors (due to shifted inverse itertion).

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