BORDERED MATRICES AND APPLICATIONS TO ERGODIC MARKOV CHAINS

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ABSTRACT

Systems of linear equations involving submatrices of singular M-matrices have been considered in the calculation of stationary distribution vectors of ergodic Markov chains. In this paper, we suggest an alternative approach using bordered matrices of the M-matrices instead. The conditioning of the approach is analysed.

1. Introduction

Consider the problem of finding the right eigenvector p corresponding to the simple zero eigenvalue of the $n \times n$ matrix A, i.e.

(1.1a) $$Ap = 0$$

subject to the scaling constraint

(1.1b) $$e^T p = 1$$

for some vector e not defficient in the left - eigenvector corresponding to the zero eigenvalue.

The problem in (1.1) arises from the calculation of the stationary distribution of an ergodic Markov chain, where the vector e in (1.1b) can be chosen to be the left-eigenvector

(1.2) $$e = (1, \ldots , 1)^T / \sqrt{n}$$

with $\|e\|_2 = 1$, and A an M-matrix. The solution vector p can then be proved to be positive.

Background information on the problem can be found in [1][2][11]-[14] [16][17][19][21]-[23][25][26][28] on M-matrices and Markov chains, and the references therein. Various numerical algorithms and applications were suggested and analysed.

The conditioning of the problem has been examined through the use of $A^{\#}$, the group inverse of A (c.f. [14][16][22]), or the smallest positive singular value of A (c.f.[1][19]).

In [1], Barlow solved the problem in (1.1) by the following algorithm:-

ALGORITHM (BARLOW [1]):-

1. Find j and k such that

(1.3) $$A = P_j \begin{pmatrix} B & y \\ z^T & \alpha \end{pmatrix} P_k^T$$

where P_i exchanges rows i and n .

(B is a submatrix of A by the deletions of the j-th row and k- column.)

2. By LU or QR decomposition, solve

(1.4) $$B\hat{x} = -y \quad .$$

3. Let $x = P_k\binom{\hat{x}}{1}$ and $p = x/(\sum_{i=1}^{n} x_i)$,

such that $\|p\|_1 = 1$, a different scaling from (1.1b).

Barlow proved that

(1.5) $$\frac{\sigma_{n-1}^{(A)}}{(|V_{kn}|^{-1}+1)(\sqrt{n}+1)} \leq \sigma_{n-1}^{(B)} \leq \sigma_{n-1}^{(A)} \quad ,$$

where $\sigma_i^{(m)}$ denotes the i-th singular value of the matrix M , for some number $|V_{kn}|$ (see [1] for details).

As $\sigma_{n-1}^{(A)}$ is a "condition number" of the problem in (1.1) (c.f. [1][19]), it is claimed from (1.5) that solving problem (1.1) or (1.4) involves the same conditioning.

The algorithm is inadequate in the following sense:-

(a) $\sigma_{n-1}^{(A)}$ only was used in reflecting the condition of the problem (1.1) , and the usual condition number

(1.6) $$s_n = \cos^{-1}(e,p) = \cos^{-1}(\Theta_n)$$

by Wilkinson [29] is not involved

(b) In addition, $\sigma_{n-1}^{(B)}$ was used to represent the conditioning of (1.4), and not the usual condition number.

(1.7) $$\kappa_2(B) = \|B\|_2.\|B^{-1}\|_2 = \sigma_1^{(B)} / \sigma_{n-1}^{(B)} \quad .$$

(c) The lower bound in (1.5) can be poor and vertually zero for large enough n or small enough $|V_{kn}|$.

(d) It may require to solve (1.4) more than once to choose P_k in algorithm to maximize $|V_{kn}|$.

In order to overcome the problems stated in (a)-(d) above, an alternative algorithm is suggested as follows:-

Solve for some vector q

(1.8) $$\tilde{A}\tilde{x} = \begin{pmatrix} A & q \\ e^T & 0 \end{pmatrix} \begin{pmatrix} x \\ \beta \end{pmatrix} = \begin{pmatrix} q \\ 1 \end{pmatrix}$$

by QR or LU decomposition, then scale x to form p according to some desired scheme, if different from (1.1b).

Note that β in (1.8) should be 1 and can serve as a check of accuracy in the algorithm.

The idea of bordering a singular matrix to yield a nonsingular one is an old one [3]. It is also related to inverse iteration and Newton's method [10][15][20][24], and has various applications, e.g. [4][5][27].

The main result of this paper is

(1.9) $$\kappa_2^2(A) \leq \kappa_2^2(\tilde{A}) \leq \mathcal{C}_1 \kappa_2^2(A) + \mathcal{C}_2$$

for some constants $\mathcal{C}_i$, which are dependent on $\cos \Theta_n$ but small under normal circumstances, and the conditioning of problem (1.1) can be represented by the quantity

(1.10) $$s_n \cdot \kappa_2(A) = \kappa_2(A) / \cos \Theta_n \quad .$$

(recall (1.6) .)

It is important at this point to stress that the assumptions that A is an M-matrix, or e is in the form of (1.2), are not essential in the investigation in this paper, except in comment (5) in Section 3.

Note that the problem (1.1) has been analysed thoroughly in the context of eigenvalue problems by various authors, especially those by Wilkinson [24][29], and all algorithms suggested (including ours) are equivalent to the inverse iteration [24][29] in some way. It is with this understanding in mind that this paper is written, and efforts have been made to relate our results to others, especially those by Wilkinson [24][29].

2. Conditioning of Problem.

From [29], s_n in (1.6) is condition number of the problem in (1.1), with $|\lambda_{n-1}|$ (the smallest non-zero eigenvalue of A, in this case the separation between the zero and non-zero spectra) appearing in the second order perturbation error bound.

In [1][19], it has been shown that $\sigma_{n-1}^{(A)}$ is a condition number of the problem in the sense that :

if $\tilde{p}$ satisfies the perturbed system

(2.1a) $\begin{cases} A\tilde{p} = r \quad , \\ e^T\tilde{p} = 1 \quad , \end{cases}$ (2.1b)

we have , for $\delta p = \tilde{p}-p$,

(2.2) $$\|\delta p\|_2 \leqq (1+\sqrt{n}\ ) \ . \ \|r\|_2 \ / \ \sigma_{n-1}^{(A)} \quad .$$

The result is comparable to that concerning $|\lambda_{n-1}|$ in [29].

By treating (1.1) as a homogeneous system of equations with constraints, we can prove the following lemma:

LEMMA 2.1. Let A be a singular $n\mathrm{x}n$ matrix of rank $n-1$. If δp satisfies (2.1), then

(2.3) $$\frac{\|\delta p\|_2}{\|p\|_2} \leqq \frac{\kappa_2(A)}{\cos\Theta_n} \cdot \frac{\|r\|_2}{\|A\|_2} \quad ,$$

with $\cos\Theta_n = \cos(e,p) = \dfrac{|e^Tp|}{\|e\|_2 . \|p\|_2}$.

Proof. From (1.1) and (2.2), one has

(2.4a) $\begin{cases} A.\delta p = r \quad , \\ e^T . \ \delta p = 0 \quad . \end{cases}$ (2.4b)

From (2.4a) ,

(2.5) $$\delta p = A^{+}r + \gamma p$$

for some constant γ, and A^{+} denotes the (1,2,3,4)- or Penrose-inverse of A [18].

Let the singular value decomposition SVD of A be

(2.6) $$A = (U_1, U_n)\begin{pmatrix}\Sigma & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}V_1^T\\ V_n^T\end{pmatrix} = U_1\Sigma V_1^T .$$

Note that $U_n = e$ and $V_n = p/\|p\|_2$,

or $p = V_n / U_n^T V_n$ from (1.1b).

Premultiply (2.5) by e^T, and using (2.4b), one has

(2.7) $$\gamma = -e^T A^{+} r .$$

Substitute γ in (2.7) back to (2.5), using the well-known expression for A^{+} [18] in terms of the SVD in (2.6),

(2.8) $$A^{+} = V_1\Sigma^{-1}U_1^{\,T} ,$$

one arrives at

(2.9) $$\delta p = V_1\Sigma^{-1}U_1^T \cdot r - U_n^T V_1\Sigma^{-1}U_1^T \cdot r \cdot p$$

$$= Q \cdot V_1\Sigma^{-1}U_1^{T} \cdot r$$

with $$Q = I - \frac{V_n U_n^T}{U_n^T V_n} .$$

It is easy to prove that $\|Q\|_2 = \cos^{-1}(\Theta_n)$ by considering the eigenvalues of QQ^T.

From (2.9), it is then proved that

$$\frac{\|\delta p\|_2}{\|p\|_2} \leq \frac{\|Q\|_2 \cdot \|\Sigma^{-1}\|_2 \cdot \|r\|_2}{\|p\|_2} \leq \frac{\kappa_2(A)}{\cos\Theta_n} \cdot \frac{\|r\|_2}{\|A\|_2}$$

from the fact that $\|\Sigma^{-1}\|_2^{-1} = \sigma_{n-1}^{(A)}$ and $\|p\|_2^{-1} \leq \|e\|_2$ from (1.1b).

Q.E.D.

Notice the appearance of $\cos\Theta_n$ in (2.3), in agreement with the results by Wilkinson [29]. Also, using $\kappa_2(A)$ instead if $\sigma_{n-1}^{(A)}$ reflects the scaling of the problem, as seen from the relative error inequality in (2.3).

In [14][16][22], $\|A^{\#}\|_2$ can be proved to be a condition number of the problem. The following lemma links up the group inverse condition number $\|A^{\#}\|_2$ with the traditional condition numbers:

LEMMA 2.2 : The group inverse $A^{\#}$ can be expressed in terms of the SVD of A in (2.6) by

(2.10) $$A^{\#} = U_1 \, (V_1^T U_1)^{-1} \, \Sigma^{-1} \, (V_1^T U_1)^{-1} \, V_1^T \quad .$$ (c.f. (2.8).)

In addition, one has

(2.11) $$\|A^{\#}\|_2 \leqq \|A^{+}\| \cos^{-2}(\Theta_n) = \left[\sigma_{n-1}^{(A)} \cdot \cos^2(\Theta_n)\right]^{-1}$$

Proof : It is easy to check that $A^{\#}$ expressed in (2.10) satisfies the conditions [16]

$$A\,A^{\#}\,A = A \,, \quad A^{\#}\,A\,A^{\#} = A^{\#} \quad \text{and} \quad A^{\#}\,A = A\,A^{\#} \quad .$$

As the group inverse $A^{\#}$ is unique for given A, $A^{\#}$ in (2.10) must be one of its expression. (See [14][16][22] for more information on $A^{\#}$.)

From (2.10) , $\|A^{\#}\|_2 \leqq \|\Sigma^{-1}\|_2 \cdot \|(V_1^T U_1)^{-1}\|_2^2$ and (2.11) is proved from the C-S decomposition [18] of $V^T U = (V_1, V_n)^T \cdot (U_1, U_n)$.

Q.E.D.

Note that a similar Lemma to Lemma 2.1 can be proved using Lemma 2.2 and the analysis in [14] .

From [6][7], the quantity $\|(V_1^T U_1)^{-1}\|_2$ can be shown to be related to the conditioning of the non-zero spectrum of A .

It is clear from Lemma 2.2 that $\|A^{\#}\|_2$ is a good condition number of the problem (1.1), as it combines the effects of the quantities $\|A^{+}\|_2$ and $\cos\Theta_n$.

A new way of calculating the group inverse $A^{\#}$ will be to use the formula (2.10), with $(V_1^T U_1)^{-1}$ constructed by an additional SVD, QR or LU decomposition. The SVD's (for A and $V^T U$) will be essential if rank determinations are critical in the calculation. (For another algorithm for calculating $A^{\#}$, see [14].)

3. Main Result.

Consider the eigenvalues of the matrix $\tilde{A}\tilde{A}^T$, where

(3.1) $$\tilde{A} = \begin{pmatrix} A & e \\ e^T & 0 \end{pmatrix} = \begin{pmatrix} U_1 & U_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \Sigma & 0 & C_1 \\ 0 & 0 & C_2 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} V_1^T & 0 \\ V_2^T & 0 \\ 0 & 1 \end{pmatrix}$$

which are $(\sigma_i^{(\tilde{A})})^2$. (c.f. (2.6).)

Equation (3.1) implies that $\tilde{A}\tilde{A}^T$ is unitarily similar to the matrix

(3.2) $$\begin{pmatrix} \Sigma & C_1 & 0 \\ 0 & C_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \Sigma & 0 & 0 \\ C_1^T & C_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \Sigma^2 + C_1 C_1^T & C_2 C_1 & 0 \\ C_2 C_1^T & C_2^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Note that $C^T C = (C_1^T , C_2) \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \|e\|_2^2 = 1$,

(3.3) $$|C_2| = \cos\Theta_n \quad \text{and} \quad \|C_1\|_2 = \sin\Theta_n \quad .$$

Consider now only the nxn submatrix M of (3.2) by deleting the last row and column. It is a rank-1 update

(3.4) $$M = \begin{pmatrix} \Sigma^2 & 0 \\ 0 & 0 \end{pmatrix} + C\,C^T \quad .$$

Using the theory for rank-1 updates [18][29], we have the following inequalities :-

$$(3.5)\quad \begin{cases} (\sigma_1^{(A)})^2 \leqq (\sigma_1^{(M)}) \leqq (\sigma_1^{(A)})^2 + 1 \;, \\ \sigma_n^{(M)} \leqq \sigma_{n-1}^{(A)} \;,\; \sigma_n^{(M)} \leqq 1 \;. \end{cases}$$

Note that, from (3.2) and (3.5) ,

$$(3.6)\quad \tilde{\sigma}_1^{(A)} = \max\,\{1,\ \sigma_1^{(M)}\} \;,\quad \tilde{\sigma}_{n+1}^{(A)} = \min\,\{1\ ,\sigma_n^{(M)}\} = \sigma_n^{(M)} \;.$$

One can prove the following lemma concerning the lower bound by $\sigma_n^{(M)}$:-

<u>LEMMA 3.1.</u>

$$(3.7)\quad (\sigma_n^{(M)})^2 \geq \frac{\cos^2\Theta_n \cdot (\sigma_{n-1}^{(A)})^2}{(\sigma_{n-1}^{(A)})^2 + (\sin\Theta_n + \cos\Theta_n)^2}$$

$$\geq \frac{\cos^2\Theta_n \cdot (\sigma_{n-1}^{(A)})^2}{(\sigma_{n-1}^{(A)})^2 + 2} \;.$$

<u>Proof:-</u> From the well-known rank-1 update of an inverse formula [18]

$$(\tilde{M} + UV^T)^{-1} = \tilde{M}^{-1} - \tilde{M}^{-1}\, U\, V^T\, \tilde{M}^{-1} \,/\, (1 + V^T\tilde{M}^{-1}U) \;,$$

the inverse of M in (3.4) equals to

$$M^{-1} = \left[\begin{array}{c|c} \Sigma^{-2} & -C_2^{-1}\Sigma^{-2}C_1 \\ \hline -C_2^{-1}\,C_1^T\,\Sigma^{-2} & C_2^{-2}(1 + C_1^T\,\Sigma^{-2}\,C_1) \end{array}\right]$$

Let $(\sigma_n^{(M)})^{-2} = \|M^{-1}\|_2 = x^T\,M^{-1}\,x$ for some x of unit length.

The properties of norms and (3.3) imply that

$$(\sigma_n^{(M)})^{-2} \leqq (\sigma_{n-1}^{(A)})^2 \cdot (1 + \tan\Theta_n)^2 + \sec^2\Theta_n \;,$$

which implies (3.7), with $\max_{\Theta}\,(\sin\Theta + \cos\Theta)^2 = 2$.

Q.E.D.

We can then prove our main result, stated in (1.9) in a slightly different form:-

THEOREM 3.2

(3.8) $\kappa_2^2(A) \leq \kappa_2^2(\tilde{A}) \leq (\mathcal{C}_1 \cdot \kappa_2^2(A) + \mathcal{C}_2) \cdot \cos^{-2}(\theta_n)$,

where (i) $\mathcal{C}_1 = 5$, $\mathcal{C}_2 = 1$ for $\sigma_1^{(A)} \geq 1$, $\sigma_{n-1}^{(A)} \leq 1$.

(ii) $\mathcal{C}_1 = (4 + (\sigma_{n-1}^{(A)})^2)$, $\mathcal{C}_2 = 1$;

or $\mathcal{C}_1 = 2$, $\mathcal{C}_2 = 3 + (\sigma_1^{(A)})^2$;

for $\sigma_1^{(A)} \geq 1$, $\sigma_{n-1}^{(A)} \geq 1$.

(iii) $\mathcal{C}_1 = 3 + 2\,(\sigma_1^{(A)})^{-2}$, $\mathcal{C}_2 = 1$;

or $\mathcal{C}_1 = 2$, $\mathcal{C}_2 = 2\,(1 + (\sigma_{n-1}^{(A)})^{-2})$;

for $\sigma_1^{(A)} \leq 1$, $\sigma_{n-1}^{(A)} \leq 1$.

Proof : From (3.5)-(3.7) , one can prove

$$\kappa_2^2(A) \leq \kappa_2^2(\tilde{A}) \leq [2 + 2(\sigma_1^{(A)})^{-2} + (\sigma_{n-1}^{(A)})\,] \cdot \kappa_2^2(A) + 1$$

$$\text{or} \quad 2\kappa_2^2(A) + 1 + 2(\sigma_{n-1}^{(A)})^{-2} + (\sigma_1^{(A)})^2 .$$

By considering the three different possible cases (i)-(iii), (3.8) follows.

Q.E.D.

Comments :-

1. Note that $\mathcal{C}_1$ and $\mathcal{C}_2$ are small, except in the pathological case when $\sigma_1^{(A)}$ and $\sigma_{n-1}^{(A)}$ are both very large (in case (ii)) or very small (in case (iii))in comparison to unity.

   In such an unlikely ill-scaled event, a scaling factor can be used to scale the problem back to case (i), when $\sigma_1^{(A)} \geq 1 \geq \sigma_{n-1}^{(A)}$.

   Such scaling factor may be estimated by techniques described in [8][9] for the estimation of condition numbers.

(2) For ill-scaled problems, or problems with small $\cos\Theta_n$, iterative refinement techniques in [27][29] may have to be used to improve the accuracy of the solution.

(3) One can choose q in (1.8) to be other vectors which is not deficient in p for the algorithm, and the discussions in this section should still hold in a loose sense, if $\cos(q,p)$ is not too small. If one is so lucky to be able to choose q nearly equal to p (the solution!) , one can replace the angle Θ_n in in (3.7) bv the value 0 . However, the factor $\cos\Theta_n$ in Lemmas 2.1 and 2.2 still remains.

(4) One may want to solve the problem for $q = e$ to obtain an approximate $\tilde{p}$, and solve the problem a second time for $q = \tilde{p}$. It is not recommended, however, as $q = e$ should provide a good solution for well-conditioned problems (with small Θ_n) , and one cannot escape from ill-conditioning, according to Lemma 2.1 .

(5) It is easy to show that $\tilde{A}$ is an M-matrix if A is one. The techniques in [11][12][13] can be used to solve the system of equations in (1.8) without pivoting, the only benefit of requiring A to be an M-matrix in this paper.

(6) For rank > 1 defficient cases, one may want to find P such that

$$\begin{cases} AP = 0 \\ E^T P = I \end{cases}$$

A similar theory to the one in this paper will hold but one has to have prior knowledge of E for the scaling of P.

4. Conclusions

A direct algorithm for solving (1.1) has been proposed. It has been proved that the conditioning of the algorithm is comparable to that of the original problem. Wilkinson's condition number for eigenvalue problem,

$s_i = \cos^{-1}(\theta_i)$, and $\kappa_2(A)$ have been shown to have important roles in the conditioning of the problem and the algorithm.

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