PARTIAL PIVOTING STRATEGIES FOR SYMMETRIC MATRICES

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Abstract

Partial pivoting strategies for the decomposition of symmetric matrices are discussed for solving symmetric (indefinite) systems of linear equations and for calculating the signature of symmetric matrices, in both the full and the sparse band cases.

Key Words: diagonal pivoting, symmetric, indefinite, linear equations, signature, sparse, band

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1. Introduction

Recently Bunch [3] and Bunch and Parlett [5] have presented a stable algorithm for solving symmetric systems of linear equations and for calculating the signature of symmetric matrices. Aasen [1] has presented a modification of the tridiagonal method of Parlett and Reid [7] for solving symmetric systems of linear equations, but which would not preserve the signature.

Let A be a symmetric matrix of order n and rank r. Let u,v be the number of positive, negative eigenvalues of A. Then $s \equiv u-v$ is the signature of A. By Sylvester's Inertia Theorem (Mirsky [6], p. 377), the rank and signature are invariant under linear transformations. Since $r = u + v$, if we know the rank and signature, then we know the number of positive, negative, and zero eigenvalues of A, and conversely.

The diagonal pivoting method of Bunch and Parlett reduces the nxn non-singular symmetric matrix A by congruences to a block diagonal matrix D, each block being of order 1 or 2. The blocks of order 2 correspond to rotations in Lagrange's method (Mirsky [6], pp. 371-374), and hence signature is preserved.

The signature of A can be obtained by inspection from D. Let D have p blocks of order 1 and $q = (n-p)/2$ blocks of order 2 (recall $r = n$). Each block of order 2 corresponds to a positive-negative pair of eigenvalues (since its determinant will necessarily be negative). If k,m of the blocks of order 1 have a positive, negative element, respectively, where $k+m = p$, then $u = k + q$, $v = m + q$, $s = k - m$. (The diagonal pivoting method can also be re-organized to take care of the case $r < n$.)

Bunch and Parlett present a complete pivoting strategy which is nearly as stable as Gaussian elimination with complete pivoting, while requiring $\frac{1}{6}n^3$ multiplications, $\frac{1}{6}n^3$ additions, and $\geq \frac{1}{12}n^3$ but $\leq \frac{1}{6}n^3$ comparisons to solve a symmetric system of linear equations of order n or to calculate the signature of a symmetric matrix of order n.

In §2 we present a partial pivoting strategy for the diagonal pivoting method requiring only n^2 comparisons with element growth bounded by $(1+1/\alpha_0)^{n-1} < (2.57)^{n-1}$, where $\alpha_0 = (1+\sqrt{17})/8$.

In §3 we discuss the tridiagonal method of Parlett and Reid [7] and Aasen [1]. It reduces the $n \times n$ symmetric matrix A by stabilized congruences to a tridiagonal form T; a partial pivoting strategy is used to stabilize the reduction. The tridiagonal system is solved by Gaussian elimination with partial pivoting. (This last step would not preserve signature.) The element growth is bounded by 2^{2n-3}.

The usefulness of Gaussian elimination with partial pivoting lies in the fact that although the bound of 2^{n-1} is reachable (Wilkinson [9], p. 212), such growth does not occur in practical problems. We leave as an open question whether such growth also does not occur for the tridiagonal method in practical problems. Parlett and Reid's version requires $\frac{1}{3}n^3$ multiplications, $\frac{1}{3}n^3$ additions, and $\frac{1}{2}n^2$ comparisons, while Aasen's modification requires $\frac{1}{6}n^3$ multiplications, $\frac{1}{6}n^3$ additions, and $\frac{1}{2}n^2$ comparisons.

We discuss the application of these methods for solving linear equations and for calculating signature when the matrix is sparse and banded.

2. A Partial Pivoting Strategy for the Diagonal Pivoting Method

A matrix A is row(column) equilibrated if all its rows (columns) have the same length in some norm; A is equilibrated if all its rows and columns have the same length in some norm.

Let A be an nxn non-singular symmetric matrix which is equilibrated in the max-norm, i.e. $\max_j |A_{ij}| = \mu_0$ for each i. (For a simple algorithm for equilibrating symmetric matrices in the max-norm, see Bunch [2].)

Let $A^{(n)} = A$, and $A^{(k)}$ be the reduced matrix of order k. (Note that if $A^{(k)}$ uses a 2x2 pivot then $A^{(k-1)}$ does not exist.)

Let $\mu_0^{(k)} = \max_{i,j} |A_{ij}^{(k)}|$. (We shall not actually calculate $\mu_0^{(k)}$.)

Let $\mu_1^{(k)} = \max_i |A_{ii}^{(k)}|, = |A_{jj}^{(k)}|$ say. We shall assume we have interchanged rows and columns so that $|A_{11}^{(k)}| = \mu_1^{(k)}$. Then let $\lambda^{(k)} = \max_i |A_{i1}^{(k)}|$. So $\lambda^{(k)} \leq \mu_0^{(k)}$, while $\lambda^{(n)} = \mu_0^{(n)} = \mu_0$.

We shall use a 1x1 pivot iff $\mu_1^{(k)} \geq \alpha\lambda^{(k)}$, where $0 < \alpha < 1$. Let m be any multiplier of $A^{(k)}$ (see [5], p. 645).

If $\mu_1^{(k)} \geq \alpha\lambda^{(k)}$, then we use $A_{11}^{(k)}$ as a 1x1 pivot. (Recall $|A_{11}^{(k)}| = \mu_1^{(k)}$.) So $|m| \leq \lambda^{(k)}/\mu_1^{(k)} \leq 1/\alpha$, while $\max_{i,j} |A_{ij}^{(k-1)}| \leq \mu_0^{(k)} + \lambda^{(k)}/\alpha \leq (1+1/\alpha)\mu_0^{(k)}$.

If $\mu_1^{(k)} < \alpha\lambda^{(k)}$, then we interchange so that $|A_{21}^{(k)}| = \lambda^{(k)}$. Let $\nu^{(k)} \equiv |A_{11}^{(k)} A_{22}^{(k)} - A_{21}^{(k)2}|$. So $\nu^{(k)} = A_{21}^{(k)2} - A_{11}^{(k)} A_{22}^{(k)} = \lambda^{(k)2} - A_{11}^{(k)} A_{22}^{(k)} \geq \lambda^{(k)2} - \mu_1^{(k)2} > (1-\alpha^2)\lambda^{(k)2}$.

Then $|m| \le \lambda^{(k)} [\mu_0^{(k)} + \mu_1^{(k)}]/\nu^{(k)}$ and $\max_{i,j} |A_{ij}^{(k-2)}| \le$

$\mu_0^{(k)} + 2\lambda^{(k)2} [\mu_0^{(k)} + \mu_1^{(k)}]/\nu^{(k)} < [1 + \frac{2}{1-\alpha}]\mu_0^{(k)}$.

As in [5], $\max_{i,j} |A_{ij}^{(k)}| \le \max \left\{ \left(1+\frac{1}{\alpha}\right)^{n-k}, \left(1+\frac{2}{1-\alpha}\right)^{\frac{n-k}{2}} \right\} \mu_0$

$\left(\max\left\{1+\frac{1}{\alpha}, \sqrt{1+\frac{2}{1-\alpha}}\right\}\right)^{n-k} \mu_0$ and

$$\min_{0<\alpha<1} \left(\max\left\{1+\frac{1}{\alpha}, \sqrt{1+\frac{2}{1-\alpha}}\right\}\right)^{n-k} = (1+\frac{1}{\alpha_0})^{n-k} < (2.57)^{n-k} ,$$

where $\alpha_0 \equiv (1+\sqrt{17})/8 \doteq 0.6404$. Thus $\max_k \max_{i,j} |A_{ij}^{(k)}| \le$

$(1+\frac{1}{\alpha_0})^{n-1} \mu_0 < (2.57)^{n-1} \mu_0$.

This bound compares favorably with that of $2^{n-1}\mu_0$ for Gaussian elimination with partial pivoting, while requiring only $\frac{1}{6}n^3$ multiplications, $\frac{1}{6}n^3$ additions, and n^2 comparisons.

No such bound exists for unequilibrated matrices.

Consider $\begin{bmatrix} \frac{1}{2}\alpha\varepsilon & \varepsilon & \varepsilon \\ \varepsilon & \frac{1}{2}\alpha\varepsilon & 1 \\ \varepsilon & 1 & \frac{1}{2}\alpha\varepsilon \end{bmatrix}$.

3. The Tridiagonal Method

The nxn symmetric matrix A is reduced to a tridiagonal form by congruences with a partial pivoting strategy. Let $A^{(k)}$ be the reduced matrix of order k. The largest off-diagonal element in the first column is brought into the (2,1) position by interchanging rows and corresponding columns. The element in the (2,1) position is then used as the pivot in the elimination.

Suppose we have interchanged rows and columns so that

$$A^{(k)} = \begin{bmatrix} A_{11}^{(k)} & A_{21}^{(k)} & \cdots & A_{k1}^{(k)} \\ A_{21}^{(k)} & A_{22}^{(k)} & \cdots & \\ \vdots & \vdots & & \\ A_{k1}^{(k)} & & & A_{kk}^{(k)} \end{bmatrix}, \quad \text{where } |A_{21}^{(k)}| = \max_{2\le i\le k} |A_{i1}^{(k)}| .$$

Let $$L_k = \left[\begin{array}{c|c|c} 1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ \hline 0 & \ell_k & I_{k-2} \end{array}\right], \quad \text{where } \ell_k = \begin{bmatrix} A_{31}^{(k)}/A_{21}^{(k)} \\ \vdots \\ A_{k1}^{(k)}/A_{21}^{(k)} \end{bmatrix}, \quad \ell_{k,i-2} = \frac{A_{i1}^{(k)}}{A_{21}^{(k)}},$$

and I_{k-2} is the identity matrix of order k-2.

Then $$A^{(k)} = L_k \left[\begin{array}{c|c|c} A_{11}^{(k)} & A_{21}^{(k)} & 0 \\ \hline A_{21}^{(k)} & A_{22}^{(k)} & m_k^t \\ \hline 0 & m_k & A^{(k-2)} \end{array}\right] L_k^t ,$$

where $m_{k,i-2} = A_{2i}^{(k)} - \ell_{k,i-2} A_{22}^{(k)}$, $3 \le i \le k$, and

$$A^{(k-2)}_{i-2,j-2} = A^{(k)}_{ij} - \ell_{k,i-2}\, A^{(k)}_{2\,j} - \ell_{k,j-2}\, m_{k,i-2} \;, \quad 3 \le i,j \le k \;.$$

Since each element of ℓ_k is bounded by 1 , $|(m_{k+1})_i| \le 2 \max|A^{(k)}_{ij}|$ and $|A^{(k-2)}_{ij}| \le 4 \max|A^{(k)}_{ij}|$. Thus element growth in the reduction to tridiagonal form is bounded by $4^{n-2} = 2^{2n-4}$.

Example.

$$A \equiv \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix} = L\,T\,L^t \;, \text{ where}$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}, \qquad T = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & -2 \\ 0 & -2 & 4 \end{bmatrix} .$$

Gaussian elimination with partial pivoting on a tridiagonal matrix at most doubles the elements ([10], p. 288; [4], pp. A3-4). Hence the total element growth is bounded by 2^{2n-3} . This bound is much larger than the bound of $(2.57)^{n-1}$ in §2. However, such large growth does not seem to occur in practice.

In this formulation, however, the tridiagonal method requires $\frac{1}{3}n^3$ multiplications and additions. In Aasen's formulation, the work is halved by successively calculating the elements in $H = TL^t$ and $A = LH$ in a certain order ([1], p. 235). Due to the partial pivoting strategy, only $\frac{1}{2}n^2$ comparisons are needed.

4. Another Approach

A third approach would be to reduce A to tridiagonal form T by stabilized congruences as in §3, and then solve the symmetric tridiagonal system by the following symmetry-preserving algorithm.

Let T be an nxn symmetric non-singular tridiagonal matrix. Let $T_{ii} = a_i$, $1 \le i \le n$, and $T_{i,i+1} = b_i = T_{i+1,i}$, $1 \le i \le n-1$. Assume $|a_i| \le \gamma$ while $\max_{2\le i\le n}|a_i|$, $\max_{1\le i\le n-1} |b_i| \le \beta$. Without loss of generality, we may assume T is irreducible and $\min_{1\le i\le n-1} |b_i| \ge \rho$.

Let us consider only the first step, which is typical. We decompose $T = MDM^t$, where M is unit lower triangular, D is block diagonal with blocks of order 1 or 2, and $D_{i+1,i} \neq 0$ iff $M_{i+1,i} = 0$.

Since T is irreducible, $b_1 \neq 0$. Let $\alpha > 0$ such that $\alpha\beta < 1$.

If $|a_1| \ge \alpha\, b_1^2$, then $a_1 \neq 0$ and we shall use a_1 as a 1x1 pivot. Then $M_{21} = b_1/a_1$, $T_{11}^{(n-1)} = a_2 - M_{21}\, b_1$, and $T_{ij}^{(n-1)} = T_{i+1,j+1}$. Thus $T^{(n-1)}$ is tridiagonal, $|M_{21}| \le \dfrac{1}{\alpha |b_1|} \le \dfrac{1}{\alpha\rho}$, $|T_{11}^{(n-1)}| \le \beta + \frac{1}{\alpha}$, while $|T_{ij}^{(n-1)}| \le \beta$ otherwise.

If $|a_1| < \alpha\, b_1^2$, then we shall use $\begin{bmatrix} a_1 & b_1 \\ b_1 & a_2 \end{bmatrix}$ as a 2x2 pivot. (Note that we make no interchanges.) Then $a_1 a_2 - b_1^2 \le$

$|a_1 a_2| - b_1^2 < b_1^2(\alpha\beta-1) < 0$ since $\alpha\beta < 1$. Thus the 2x2 block corresponds to a positive-negative pair of the signature, and $|a_1 a_2 - b_1^2| > b_1^2(1-\alpha\beta) > 0$.

Now $M_{31} = -b_1 b_2/(a_1 a_2 - b_1^2)$, $M_{32} = a_1 b_2/(a_1 a_2 - b_1^2)$, $T_{11}^{(n-2)} = a_3 - M_{32} b_2$, and $T_{ij}^{(n-2)} = T_{i+2,j+2}$ otherwise. Thus $T^{(n-2)}$ is tridiagonal, $|M_{31}| \le |b_2|/[|b_1| (1 - \alpha\beta)] \le \frac{\beta}{\rho(1-\alpha\beta)}$, $|M_{32}| \le \alpha\beta/(1-\alpha\beta)$, $|T_{11}^{(n-2)}| \le \beta/(1-\alpha\beta)$, while $|T_{ij}^{(n-2)}| \le \beta$ otherwise.

We see that the bounds on the elements of $T^{(n-1)}$ for a 1x1 and $T^{(n-2)}$ for 2x2 are independent of the bound γ on $|a_1|$.

The pattern continues throughout all the reduced matrices. Hence we conclude: each matrix $T^{(k)}$ is tridiagonal, $|T_{11}^{(k)}| \le \max\{\beta + 1/\alpha, \beta/(1-\alpha\beta)\}$, while $|T_{ij}^{(k)}| \le \beta$ otherwise.

Now $\min\limits_{0<\alpha<1/\beta} \max\{\beta + 1/\alpha, \beta/(1 - \alpha\beta)\} = (\frac{3+\sqrt{5}}{2})\beta$ and is achieved by $\alpha = \frac{\sqrt{5}-1}{2\beta}$.

We shall need an n-vector array to record the pivotal selection. We set pivot[k] = N, where N is a fixed integer greater than $\frac{\beta}{\rho(1-\alpha\beta)}$, if we use a 1x1 pivot for $T^{(k)}$. Otherwise set pivot[k] = the determinant of the 2x2 pivot (necessarily negative) and pivot[k-1] = $M_{n-k+3,n-k+1}$. Then we need only 2n storage locations to store the rest of M and D (these we write over T). Thus we need only 3n storage locations for this algorithm when applied to a tridiagonal matrix.

Thus this third approach requires $\frac{1}{6}n^3$ multiplications, $\frac{1}{6}n^3$ additions, and $\frac{1}{2}n^2$ comparisons. Here $\beta \leq 2^{2n-4}$, so element growth is bounded by $(3+\sqrt{5})2^{2n-5}$. Now signature is also preserved.

5. Band Linear Equations

Consider $Ax = b$, where $A \in \mathcal{G}_n^m = \{M: M$ is an $n \times n$ non-singular matrix of band width $2m+1$, i.e. $M_{ij} = 0$ for $|i-j| > m\}$.

Let $A^{(n)} = A$; let $B(n) = \sup\limits_{A \in \mathcal{G}_n^m} \{\max\limits_k \max\limits_{i,j} |A_{ij}^{(k)}| : A^{(k)}$ is the reduced matrix of order $k\}$; and let $B'(n)$ be as above, but with the restriction that $A = A^t$.

If the LU decomposition of A exists, then the band pattern is preserved, i.e. L is unit lower triangular with $L_{ij} = 0$ for $i-j > m$ and U is upper triangular with $U_{ij} = 0$ for $j-i > m$. Thus only $(2m+2)n$ storage and $(m^2+3m+1)n$ multiplications are needed to solve $Ax = b$. In general, this is unstable, i.e. $B(n) = \infty$. If A is required to be diagonally dominant, i.e. $|A_{jj}| \geq \sum\limits_{i \neq j} |A_{ij}|$ for $1 \leq j \leq n$, then $B(n) = 2$ (Wilkinson [10], p. 288). If A is tridiagonal, then $m = 1$ and $4n$ storage and $5n$ multiplications are needed to solve $Ax = b$.

Using Gaussian elimination with partial pivoting requires $(3m + 3)n$ storage and $(2m^2 + 4m + 1)n$ multiplications to solve $Ax = b$. This is quite stable; in fact, Wilkinson [8] has shown that $B(n) \leq 2^{2m-1} - (m-1)2^{m-2}$ in this case. Note that the bound is independent of n. The bound is sharp for small m.

If A is tridiagonal ($m = 1$), then Gaussian elimination with partial pivoting requires $6n$ storage and $7n$ multiplications; here $B(n) = 2$. If A is 5-diagonal ($m = 2$), then $9n$ storage and $17n$ multiplications are required; and $B(n) = 7$.

However, Gaussian elimination with partial pivoting destroys symmetry. Let us try to preserve symmetry.

If A is also positive definite, we may use the Cholesky decomposition ([9];(m+2)n storage, $(\frac{1}{2}m^2 + \frac{7}{2}m + 1)n$ multiplications, and n root reciprocals) or symmetric Gaussian elimination (i.e. LDL^t[9];(m+2)n storage and $(\frac{1}{2}m^2 + \frac{7}{2}m + 1)n$ multiplications).

These methods, however, should not be used when A is indefinite ([5], pp. 643-645).

The diagonal pivoting method with the partial pivoting strategy of §3 would preserve symmetry, but the bandwidth could double at each step. The symmetry preserving algorithm of §4 would preserve symmetry of a tridiagonal matrix. However, if p is the number of 1x1 pivots used, then 4n + p multiplications are required for the decomposition in contrast to 4n for Gaussian elimination with partial pivoting. Solving a set of linear equations requires 9n-p and 7n multiplications, respectively. Clearly, the above would be preferable to Gaussian elimination with partial pivoting only in the cases where storage is crucial.

6. Signature of Symmetric Band Matrices

The diagonal pivoting method with the partial strategy in §2 also preserves signature, but as noted in §5 the bandwidth could double at each step.

The algorithm for tridiagonal matrices in §4 preserves the signature of tridiagonal matrices. It requires $4n + p$ multiplications, where p is the number of 1x1 pivots used.

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