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STABILITY OF A PIVOTING STRATEGY FOR PARALLEL GAUSSIAN ELIMINATION *

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Abstract.

Gaussian elimination with partial pivoting achieved by adding the pivot row to the kth row at step k, was introduced by Onaga and Takechi in 1986 as a means for reducing communications in parallel implementations. In this paper it is shown that the growth factor of this partial pivoting algorithm is bounded above by $\mu_n < 3^{n-1}$, as compared to 2^{n-1} for the standard partial pivoting. This bound μ_n, close to 3^{n-2}, is attainable for a class of near-singular matrices. Moreover, for the same matrices the growth factor is small under partial pivoting.

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Key words: Gaussian elimination, parallel algorithm, growth factor, stability.

1 Introduction.

The reduction of a system of equations $Ax = b$ to upper triangular form, $Ux = d$, by Gaussian elimination (GE) with partial pivoting (GEPP) is well known [1]. Suppose that the matrices at each step of the Gaussian elimination with pivoting are denoted by $A^{(k)}$, $k = 0, 1, \ldots, n-1$, where $A^{(0)} = A$, and the rows of $A^{(k)}$ are denoted by the row vectors $\mathbf{a}_l^{(k)}$, $l = 1, 2, \ldots, n$. At the kth pivoting stage GEPP proceeds by exchanging row $\mathbf{a}_k^{(k-1)}$ with pivot row $\mathbf{a}_{l_k}^{(k-1)}$, where $l_k > k$, the index of the pivot row at step k, is chosen to guarantee that the multipliers

$$m_{ik} = a_{ik}^{(k-1)}/a_{kk}^{(k)}, \quad i > k,$$

are bounded by one in modulus. Note, here and throughout, the subscript denotes the row index and the superscript (k) indicates the value of that quantity for the kth reduction in the Gaussian elimination. In a serial implementation of GEPP the "exchange" of rows is recorded as an index permutation, while in parallel implementations, physical exchange of elements of A between processors will actually be required to implement GEPP. The communication cost associated with this exchange may be a limiting factor in the global efficiency of the parallel implementation, particularly if bidirectional communication is not possible. Onaga and Takechi [4] proposed a modification of the pivoting strategy,

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employing uni-directional communication; Gaussian elimination with partial pivoting by adding (GEPPA). At the pivoting phase in GEPPA the pivot row $\mathbf{a}_{l_k}^{(k-1)}$ is identified, and then, if $l_k > k$ rather than switching rows $\mathbf{a}_{l_k}^{(k-1)}$ and $\mathbf{a}_k^{(k-1)}$ as in GEPP, $\mathbf{a}_{l_k}^{(k-1)}$ is "added" to $\mathbf{a}_k^{(k-1)}$ according to

$$\mathbf{a}_k^{(k)} = \mathbf{a}_k^{(k-1)} + \sigma_k \mathbf{a}_l^{(k-1)}, \qquad \sigma_k = \text{sign}(a_{l_k k}^{(k-1)} a_{kk}^{(k-1)}). \tag{1.1}$$

Here, if $a_{kk}^{(k-1)} = 0$, the convention sign $(0) = 1$ is adopted. In this way the multipliers are guaranteed to be bounded by one in modulus. Moreover, just as GEPP corresponds to the LU factorization of a permuted matrix PA, where P is a permutation matrix, it can be shown that GEPPA corresponds to the LU factorization of a matrix RA. The matrix R is unit upper triangular with non-zero entries given by

$$r_{kl} = \sigma_k 1,$$

and L is unit lower triangular with $|l_{kj}| \leq 2$ for $1 \leq j < k < n$ and $|l_{nj}| \leq 1$ for $1 \leq j < n$.

A measure of the stability of algorithms for GE is given by the growth factor which measures the growth in the elements of the reduced matrices $A^{(k)}$, with respect to those of A:

Definition 1.1. *The growth factor, ρ, is defined to be the ratio of the largest element (in magnitude) over all reduced matrices $A^{(k)}$, $k = 1, \ldots, n-1$, to the largest element of A,*

$$\rho = \frac{\max_k(\max_{i,j} |a_{ij}^{(k)}|)}{\max_{i,j} |a_{ij}|}.$$

The bound for the growth factor, ρ_{GEPP}, under the standard partial pivoting,

$$\rho_{GEPP} \leq 2^{n-1}$$

is well known [1]. It is not difficult to show from (1.1) that the growth in max norm of rows between matrices $A^{(k-1)}$ and $A^{(k)}$ is determined by

$$\|\mathbf{a}_i^{(k)}\|_\infty \leq \begin{cases} \|\mathbf{a}_i^{(k-1)}\|_\infty, & \text{if } i < k, \\ \|\mathbf{a}_k^{(k-1)}\|_\infty + \|\mathbf{a}_{l_k}^{(k-1)}\|_\infty, & \text{if } i = k, \\ \max(\|\mathbf{a}_{l_k}^{(k-1)}\|_\infty, \|\mathbf{a}_k^{(k-1)}\|_\infty), & \text{if } i = l_k, \\ \|\mathbf{a}_i^{(k-1)}\|_\infty + \|\mathbf{a}_{l_k}^{(k-1)}\|_\infty + \|\mathbf{a}_k^{(k-1)}\|_\infty, & \text{if } k+1 \leq i \leq n,\ i \neq l_k. \end{cases} \tag{1.2}$$

Thus the elements in the reduced matrices $A^{(k)}$, with respect to those of A, grow by at most a factor of 3 each step. Moreover, at the last step of the reduction the factor 3 cannot be achieved. We thus arrive at the following result, which provides the upper bound for ρ_{GEPPA}.

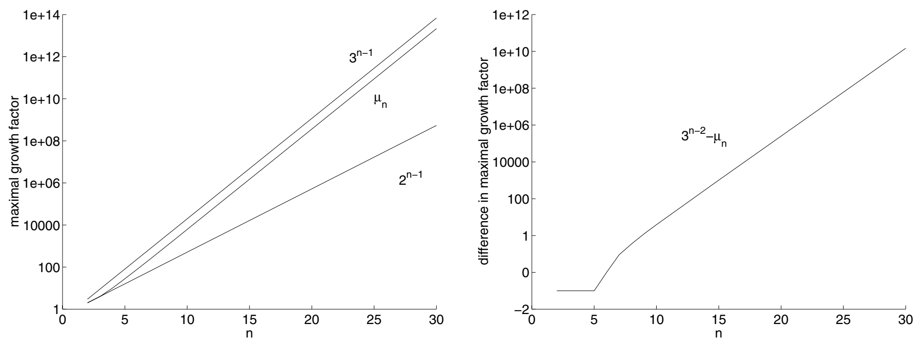

Figure 1.1: Comparison of maximal growths (left), and difference between 3^{n-2} and μ_n (right).

THEOREM 1.1. *The growth factor, ρ_{GEPPA}, for partial pivoting with addition satisfies*

$$\rho_{GEPPA} < 3^{n-1}.$$

The attainable bound μ_n on ρ_{GEPPA} [3] satisfies $\mu_n < 3^{n-2}$, $n \geq 6$, as illustrated in Figure 1.1. Moreover, this compares favorably with the bound 4^{n-1}, shown by Sorensen, [5], for pairwise pivoting.

The purpose of this paper is to investigate the stability of the GEPPA algorithm via a numerical study of the growth factor for GEPPA. Although the presented theoretical results demonstrate that GEPPA is potentially worse than GEPP with regards to backwards stability properties, as measured by larger growth factors, it is critical to assess the algorithm for average case matrices, and to determine whether the upper bound is achievable. We demonstrate in Section 2 that, although a class of matrices can be found for which the upper bound is achieved, on the average, the growth factors achieved by GEPPA and GEPP are comparable. Moreover, examples have been found for which $\rho_{GEPPA} < \rho_{GEPP}$.

2 Numerical results.

The class of matrices for which μ_n can be obtained when GEPPA is applied, is determined by first taking a singular matrix and then modifying its entries by machine epsilon so as to force non-singularity, [3]. From the verification of (1.2) it is apparent that for maximal growth the multipliers should satisfy $m_{ik} = \pm 1$. Hence, if we choose $\mathbf{a}_{ik}^{(k-1)} = \tau_i \mathbf{a}_{l_k k}^{(k-1)}$ with $\tau_i = \pm 1$, the updates given by

$$\begin{aligned} &\mathbf{a}_k^{(k)} = \mathbf{a}_{l_k}^{(k-1)} + \sigma_k \mathbf{a}_k^{(k-1)}, \\ (2.1)\qquad &\mathbf{a}_i^{(k)} = \mathbf{a}_i^{(k-1)} - \tau_i \mathbf{a}_{l_k}^{(k-1)} - \tau_i \sigma_k \mathbf{a}_k^{(k-1)} \quad \text{if } i \neq l_k, \quad \text{and } i > k, \\ &\mathbf{a}_{l_k}^{(k)} = -\sigma_k \mathbf{a}_k^{(k-1)} \quad \text{if } i = l_k, \end{aligned}$$

provide maximum growth, and $\mathbf{a}_i^{(k-1)}$ can be defined backwards from $\mathbf{a}_k^{(k)}$. Thus maximal growth in the entries of $A^{(k)}$ can be achieved by setting $a_{l_k k} = 1 + \eta$ with

η the order of machine epsilon and the diagonal entries set to η. For example the matrix obtained in this way for $n = 10$ is given by

$$\begin{pmatrix} \eta & -1 & -1 & -1 & 1 & -\eta & 1 & 1+\eta & 1 & 1 \\ -1 & \eta & -1 & -1 & 1 & -(1+\eta) & -1 & -(1+\eta) & -1 & 1 \\ -1 & -1 & \eta & -1 & 1 & 1 & -\eta & -1 & 1 & 1 \\ -1 & -1 & -1 & \eta & 1 & 1 & -(1+\eta) & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & \eta & -1 & -1 & -\eta & 1 & -1 \\ 1+\eta & 1 & 1 & 1 & -1 & \eta & -1 & -(1+\eta) & -1 & 1 \\ -1 & -1 & 1+\eta & 1 & -1 & -1 & \eta & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1+\eta & 1 & 1 & \eta & -1 & -1 \\ -1 & -1 & -1 & 1+\eta & -1 & -1 & 1+\eta & -1 & 1 & 1 \\ -1 & 1+\eta & 1 & 1 & -1 & 1+\eta & 1 & 1+\eta & 1 & 1 \end{pmatrix}.$$

The growth of coefficients in matrices determined in this way was compared under elimination by GEPP and GEPPA. The results are presented in Table 2.1. The condition number $\kappa_2 = \|A\|_2\|A^{-1}\|_2$ is also reported. From these results it can be concluded that ρ_{GEPP} small does not imply ρ_{GEPPA} small, or equivalently, that ρ_{GEPPA} large does not require ρ_{GEPP} large also. Not reported are the tests for the same matrices but using pairwise pivoting. In this case there was little appreciable difference in the size of the growth factor between pairwise and partial pivoting.

Table 2.1: Growth factor for matrix generated by equations (2.1).

n	$\log_{10}(\rho_{GEPP})$	$\log_{10}(\rho_{GEPPA})$	$\log_{10}(3^{n-2})$	$\|A\|_2\|A^{-1}\|_2$
5	0.45	1.45	1.43	1.87
10	0.63	3.79	3.82	3.77
25	0.98	10.95	10.97	10.00
50	1.18	22.87	22.90	20.69
100	1.34	46.73	46.76	42.03

Results shown in Table 2.2 indicate that GEPPA, for n larger than 30, is not accurate for systems defined by (2.1), while GEPP is still accurate up to $n = 100$. As a measure of the backward stability of the algorithms we also calculated the difference, E, of the computed factorization as compared to A, namely, for GEPP $E = P^{-1}(LU) - A$, and for GEPPA $E = R^{-1}(LU) - A$. Not surprisingly $\|E\|$ is very large when the growth factor is also large, indicating that the large growth factor does show backwards instability.

It was argued by Trefethen and Schreiber [6] that, on the average, systems of equations which occur in real applications can be considered to be sets of randomly distributed real numbers. Thus to assess whether the bound derived for ρ_{GEPPA} is pessimistically high for such systems, the accuracy of GEPPA was tested using random matrices generated according to a uniform distribution. The growth factors are reported in Table 2.3. Additional numerical results are presented in [2]. We observe here that $\rho_{GEPP} < \rho_{GEPPA} << n$ and

Table 2.2: Solving $Ax = b$, A as described by (2.1), $\hat{x}$ the computed solution, b calculated from the randomly generated exact solution x.

	$\|x - \hat{x}\|/\|x\|$		$\|E\|$	
N	GEPP	GEPPA	GEPP	GEPPA
5	2.7223 e−16	1.0889 e−15	1.1102 e−16	2.2204 e−16
10	2.4474 e−16	1.8509 e−13	7.2585 e−16	3.2156 e−13
25	1.5938 e−15	2.2737 e−06	2.4576 e−15	2.1663 e−05
30	1.6896 e−15	4.3099 e−04	3.2091 e−15	2.4414 e−03
40	2.3554 e−15	6.7621 e+01	3.9833 e−15	8.4853 e+00
50	5.3660 e−15	5.6945 e+05	5.5730 e−15	7.4146 e+05
100	1.3661 e−14	2.5465 e+30	9.0809 e−15	6.0446 e+23

Table 2.3: Average growth factors from 50 uniformly distributed matrices.

N	ρ_{GEPP}	ρ_{GEPPA}	Ratio
4	1.0144	1.4645	1.4437
8	1.2049	1.6865	1.3997
16	1.7948	2.0618	1.1488
32	2.8689	3.8643	1.3470
64	4.6757	5.3944	1.1537
128	7.7762	8.4940	1.0923
256	11.8851	14.6088	1.2292
512	19.0832	20.7663	1.0882

$\rho_{GEPPA} \approx \rho_{GEPP}$, demonstrating that the stability of GEPPA is similar to that of GEPP. In Table 2.4 we give the growth factors of 5 matrices of size 16 with entries generated randomly with a uniform distribution. We see that in two cases $\rho_{GEPP} > \rho_{GEPPA}$ occurs. Hence we cannot conclude from the average case that necessarily $\rho_{GEPP} \leq \rho_{GEPPA}$. Still our results show that, on the average, the growth factors from GEPPA are larger; see [2].

Not all matrices, however, exhibit average case behavior. In particular, Wright [7] presented a set of matrices for which the growth factors are large. These matrices arise from the solution of a two-point boundary value problem, and are

Table 2.4: Growth factors for 5 uniformly distributed matrices of dimension 16×16.

ρ_{GEPP}	2.42	1.63	1.51	1.94	1.31
ρ_{GEPPA}	1.78	1.97	3.65	1.92	1.69

Table 2.5: Growth factors and condition numbers of (2.2) with $h = 0.02$.

N	ρ_{GEPP}	ρ_{GEPPA}	Ratio	$\|A\|_2\|A^{-1}\|_2$
8	1.14 e+00	1.63 e+00	1.427479	4.360403
24	1.32 e+00	1.63 e+00	1.229815	22.27574
50	2.32 e+00	4.60 e+00	1.978920	48.74113
100	1.10 e+01	3.76 e+01	3.425457	75.37583
200	3.87 e+02	1.47 e+03	3.807935	90.52391
400	5.39 e+05	2.06 e+06	3.819086	96.62072
512	3.11 e+07	1.19 e+08	3.819094	97.78428

of the form

$$\begin{bmatrix} I & & & & I \\ -e^{Mh} & I & & & \\ & -e^{Mh} & I & & \\ & & \ddots & \ddots & \\ & & & -e^{Mh} & I \end{bmatrix} \tag{2.2}$$

with h the time step and $e^{Mh} = I + Mh$. We compared the growth factors from the two different kinds of pivoting when

$$M = \begin{bmatrix} -10 & -19 \\ 19 & 30 \end{bmatrix}.$$

Unreasonably large growth was found for both methods. The growth factors for GEPPA, however, are larger, up to a factor of four, than those for partial pivoting; see Table 2.5.

3 Conclusions.

The stability of a parallel mechanism for carrying out partial pivoting has been investigated both theoretically and numerically. Theoretical results demonstrate that the upper bound on the growth factor under the parallel strategy, GEPPA, may approach 3^{n-2}, as compared to 2^{n-1} for partial pivoting. Although neither of these bounds is actually acceptable for accurate solutions of systems of equations, it has been recognized that the real issues are whether the bound is not only achievable but also likely to be achieved for the average case situations. In this case the bound is achievable, but for randomly generated matrices the growth under the new partial pivoting is comparable to, and can be less than, growth under partial pivoting. Thus, there is no reason to conclude that GEPPA will be significantly worse in practice than GEPP.

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