

On the Skeel condition number, growth factor and pivoting strategies for Gaussian elimination*

J.M. Peña

1 Introduction

Gaussian elimination (GE) with a given pivoting strategy, for nonsingular matrices $A = (a_{ij})_{1 \leq i, j \leq n}$, consists of a succession of at most $n - 1$ major steps resulting in a sequence of matrices as follows:

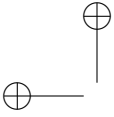
$$A = A^{(1)} \longrightarrow \tilde{A}^{(1)} \longrightarrow A^{(2)} \longrightarrow \tilde{A}^{(2)} \longrightarrow \dots \longrightarrow A^{(n)} = \tilde{A}^{(n)} = U, \quad (1)$$

where $A^{(t)} = (a_{ij}^{(t)})_{1 \leq i, j \leq n}$ has zeros below its main diagonal in the first $t - 1$ columns. The matrix $\tilde{A}^{(t)} = (\tilde{a}_{ij}^{(t)})_{1 \leq i, j \leq n}$ is obtained from the matrix $A^{(t)}$ by reordering the rows and/or columns $t, t + 1, \dots, n$ of $A^{(t)}$ according to the given pivoting strategy and satisfying $\tilde{a}_{tt}^{(t)} \neq 0$. To obtain $A^{(t+1)}$ from $\tilde{A}^{(t)}$ we produce zeros in column t below the *pivot element* $\tilde{a}_{tt}^{(t)}$ by subtracting multiples of row t from the rows beneath it. If P and/or Q are permutation matrices such that the Gaussian elimination of $B = PAQ$ can be performed without row exchanges, then the first row of $\tilde{A}^{(t)}[t, \dots, n]$ coincides with the first row of $B^{(t)}[t, \dots, n]$, and the other rows coincide up to the order. If $B = P^T A P$, we say that we have performed *symmetric pivoting*.

The growth factor is an indicator of stability of Gaussian elimination. The classical growth factor of an $n \times n$ matrix $A = (a_{ij})_{1 \leq i, j \leq n}$ is the number

$$\rho_n^W(A) := \frac{\max_{i,j,k} |a_{ij}^{(k)}|}{\max_{i,j} |a_{ij}|}$$

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In p. 398 of [1], Amodio and Mazzia have introduced the growth factor

$$\rho_n(A) := \frac{\max_k \|A^{(k)}\|_\infty}{\|A\|_\infty}.$$

and have shown its nice behaviour for error analysis of Gaussian elimination.

Conditioning is another important concept to be considered in such error analysis. The traditional condition number of a matrix A with respect to the norm $\|\cdot\|_\infty$ is given by

$$\kappa(A) := \|A\|_\infty \|A^{-1}\|_\infty.$$

Given a matrix $B = (b_{ij})_{1 \leq i, j \leq n}$, we shall denote by $|B|$ the matrix of absolute values of the entries of B . If we write $A \leq B$, it means $a_{ij} \leq b_{ij}$ for all i, j . Let us denote by I the identity matrix.

The Skeel condition number (cf. [15]) of a matrix A is defined as

$$\text{Cond}(A) = \||A^{-1}| |A|\|_\infty.$$

Let us mention two nice properties of $\text{Cond}(A)$. The Skeel condition number of a matrix A is less than or equal to $\kappa(A)$ and it can be much smaller. In contrast with $\kappa(A)$, $\text{Cond}(A)$ is invariant under row scaling.

In Section 2 we characterize the matrices with minimal Skeel condition number and we recall the Skeel condition number of some classes of triangular matrices. In Section 3 we analyze the stability properties of several pivoting strategies, taking into account the previous growth factors and condition numbers. We also consider special classes of matrices such as sign-regular matrices and totally positive matrices.

2 Bounds for the Skeel condition number

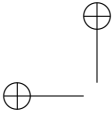
Let us recall [7] that a matrix with the same zero pattern as a permutation matrix is called a *generalized permutation matrix*. These matrices are also called monomial matrices and they are precisely the matrices with minimal Skeel condition number, as the following result shows.

Proposition 1. *A matrix satisfies $\text{Cond}(A) = 1$ if and only if A is a generalized permutation matrix.*

Proof. Clearly, any generalized permutation matrix A satisfies $\text{Cond}(A) = 1$. For the converse, let us assume that $\text{Cond}(A) = 1$. Then

$$1 = \||A^{-1}| |A|\|_\infty$$

and, since $|A^{-1}| |A| \geq |A^{-1}A| = I$, we deduce that the previous inequality must be an equality. Then we can conclude that $|A^{-1}|, |A|$ are two nonnegative matrices and $|A^{-1}| = |A|^{-1}$. Hence $|A|$ is a nonnegative matrix with nonnegative inverse and then it is well known (cf. Lemma 1.1 of [7]) that it is a generalized permutation matrix. So, the same property is inherited by A . \square



Now let us focus on the condition number of some special triangular matrices T . In Proposition 2 of [13] we proved the following result.

Proposition 2. *If $U = (u_{ij})_{1 \leq i, j \leq n}$ is a nonsingular upper triangular matrix and r a positive real number such that $r|u_{ii}| \geq |u_{ij}|$ for all $j > i$, then $\text{Cond}(U) \leq 2(1+r)^{n-1}$.*

The particular case $r = 1$ gives the following result, which had been proved in Lemma 8.6 of [5]:

Proposition 3. *If $U = (u_{ij})_{1 \leq i, j \leq n}$ is a nonsingular upper triangular matrix such that $|u_{ii}| \geq |u_{ij}|$ for all $j > i$, then $\text{Cond}(U) \leq 2^n$.*

If we impose the stronger requirement of diagonal dominance by rows, we can get the following result which corresponds to Theorem 2.1 of [10].

Proposition 4. *Let $T = (t_{ij})_{1 \leq i, j \leq n}$ be a triangular matrix which is diagonally dominant by rows. Then $\text{Cond}(T) \leq 2n - 1$.*

If the diagonal dominance of the $n \times n$ triangular matrix is strict, we even can find a bound for the Skeel condition number which is independent of n , as has been shown in Corollary 3.3 of [12]:

Proposition 5. *Let $U = (u_{ij})_{1 \leq i, j \leq n}$ be an upper triangular matrix which is strictly diagonally dominant by rows and let $p := \min_{1 \leq i \leq n} \{|u_{ii}| / \sum_{j=i}^n |u_{ij}|\}$. Then*

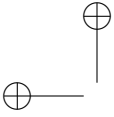
$$\text{Cond}(U) \leq \frac{1}{2p - 1}.$$

In the next section we shall show pivoting strategies leading to triangular matrices satisfying the previous properties.

3 On the stability of some pivoting strategies

GE with partial pivoting (PP) is often remarkably stable (see [17]). Let us observe that the lower triangular matrices associated to PP satisfy Proposition 3. Nevertheless, in some special cases is not good enough and we can consider other pivoting strategies. A classical (although expensive in computational cost) alternative is complete pivoting (CP), which leads to lower and upper triangular matrices satisfying Proposition 3.

On the other hand, PP is not backward stable for Gauss-Jordan elimination (GJE), as one can see in [16], [6]. In [13] we defined a pivoting strategy which is simultaneously backward stable for Gauss and Gauss Jordan elimination and which has been called double partial pivoting (DPP). Given the matrix $A^{(t)}$ in (1), let p be the first row index such that $|a_{pt}^{(t)}| = \max_{t \leq i \leq n} \{|a_{it}^{(t)}|\}$ and let p_t be the first



column index satisfying $|a_{pp_t}^{(t)}| = \max_{t \leq j \leq n} \{|a_{pj}^{(t)}|\}$. Then DPP chooses $a_{pp_t}^{(t)}$ as the t th pivot. The cost of DPP is twice the cost of PP. Observe that DPP leads to upper triangular matrices satisfying Proposition 3. Furthermore, from Proposition 3 of [13], one can derive $\rho_n(A) \leq 2^n$.

Rook's pivoting strategy (RP) selects each pivot to have maximal absolute value over both the row and column in which it lies (see [14]). So, RP leads to lower and upper triangular matrices satisfying Proposition 3. It has been shown in [4] that the growth factor of this strategy satisfies $\rho_n^W(A) \leq 1.5n^{\frac{3}{4} \log n}$. This bound grows only slightly faster than that of CP but it is much smaller than that of PP. The cost of RP varies between twice the cost of PP and the full cost of CP, although it was shown in [14] that the expected cost in a serial environment is about three times the cost of PP. As remarked in p. 358 of [14], PP selects a pivot that is maximal in its row as well as in its column with probability at least $1/2$. In [13] it is shown that DPP selects a pivot that is maximal in its row as well as in its column with probability at least $5/6$.

Let us now consider scaled partial pivoting strategies, that is, strategies which incorporate row scaling implicitly. Given $k \in \{1, 2, \dots, n\}$, let α, β be two increasing sequence of k positive integers less than or equal to n . Then we denote by $A[\alpha|\beta]$ the $k \times k$ submatrix of A containing rows numbered by α and columns numbered by β . Let $A[\alpha] := A[\alpha|\alpha]$. Let $r_i^{(t)}$ (resp., $\tilde{r}_i^{(t)}$) denote the i th row ($t \leq i \leq n$) of the submatrix $A^{(t)}[1, \dots, n|t, t+1, \dots, n]$ in (1) (resp., $\tilde{A}^{(t)}[1, \dots, n|t, t+1, \dots, n]$). A row (resp., symmetric) scaled partial pivoting strategy for the norm $\|\cdot\|_1$ consists in an implicit scaling by the norm $\|\cdot\|_1$ followed by partial (resp., symmetric and partial) pivoting. For each t ($1 \leq t \leq n-1$), these strategies look for an integer \hat{i}_t ($t \leq \hat{i}_t \leq n$) such that

$$p_t = \frac{|a_{\hat{i}_t t}^{(t)}|}{\|r_{\hat{i}_t}^{(t)}\|_1} = \max_{t \leq i \leq n} \frac{|a_{it}^{(t)}|}{\|r_i^{(t)}\|_1}$$

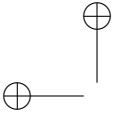
$$\text{(resp., } p_t = \frac{|a_{\hat{i}_t \hat{i}_t}^{(t)}|}{\|\tilde{r}_{\hat{i}_t}^{(t)}\|_1} = \max_{t \leq i \leq n} \frac{|a_{ii}^{(t)}|}{\|\tilde{r}_i^{(t)}\|_1} \text{)}.$$

In [8] it is shown that scaled partial pivoting strategies lead to upper triangular matrices with nice properties with respect to the Skeel condition number. Moreover, in Theorem 2.2 of [10] it was shown that if there exists a permutation matrix P such that the LU -factorization of the matrix $B = PA$ satisfies

$$|LU| = |L||U|, \tag{2}$$

then it corresponds to any row scaled partial pivoting strategy for a strict monotone vector norm. On the other hand, if (2) holds then we obtain that the growth factors $\rho_n^W(A)$ and $\rho_n(A)$ are minimal (i.e., their value is 1) for a pivoting strategy associated to P , due to the following result (which corresponds to Proposition 5.1 of [12]):

Proposition 6. *Let $B = (b_{ij})_{1 \leq i, j \leq n}$ be a nonsingular matrix. If the LU -factorization of B satisfies (2), then $|b_{ij}^{(k)}| \leq |b_{ij}|$ for all i, j, k .*



In contrast with the well known bound $\rho_n^W(A) \leq 2^{n-1}$ when partial pivoting is applied to a nonsingular $n \times n$ matrix, we cannot obtain a similar bound for $\rho_n^W(A)$ when we apply a scaled partial pivoting strategy. However, if we consider the growth factor $\rho_n(A)$ and apply either partial pivoting or the scaled partial pivoting strategy for the norm $\|\cdot\|_1$, then we get in both cases $\rho_n(A) \leq 2^{n-1}$ (see Theorem 5.1 of [1] for partial pivoting and Corollary 4.2 of [12] for the scaled partial pivoting strategy for the norm $\|\cdot\|_1$).

A disadvantage of scaled partial pivoting strategies is their high computational cost: $\mathcal{O}(n^3)$ elementary operations. However, as we shall now recall, for important classes of matrices these strategies can be implemented without computational cost or with less computational cost than partial pivoting, and they present better stability properties than partial pivoting. So let us now introduce some classes of matrices and pivoting strategies which are closely related to scaled partial pivoting strategies.

An $n \times m$ matrix A is *sign-regular* if, for each k ($1 \leq k \leq \min\{n, m\}$), all $k \times k$ submatrices of A have determinant with the same nonstrict sign. The interest of these matrices comes from their characterizations as variation-diminishing linear maps: the number of sign changes in the consecutive components of the image of a vector is bounded above by the number of sign changes in the consecutive components of the vector (cf. theorems 5.3 and 5.6 of [2]).

In [9] it was introduced a pivoting strategy for sign-regular matrices which was called *first-last pivoting* due to the fact that we choose as pivot row at each step of GE either the first or the last row among all possible rows. It presented a very well behaviour with respect to GE. We now recall the criterium of the *first-last pivoting* strategy to choose the first row of $\tilde{A}^{(t)}[t, \dots, n]$ (see (1)). If $a_{tt}^{(t)} = 0$, we choose the last row of $A^{(t)}[t, \dots, n]$. If $a_{tt}^{(t)} \neq 0$, we compute the determinant

$$d_1 := \det A^{(t)}[t, t+1].$$

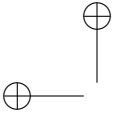
If d_1 is strictly positive (resp., negative), we choose the first (resp., last) row of $A^{(t)}[t, \dots, n]$. If $d_1 = 0$, we compute the determinant

$$d_2 := \det A^{(t)}[t, n|t, t+1].$$

If d_2 is strictly positive (resp., negative), we choose the first (resp., last) row of $A^{(t)}[t, \dots, n]$. In any case, the remaining rows of $\tilde{A}^{(t)}[t, \dots, n]$ are placed in the same relative order they have in $A^{(t)}[t, \dots, n]$.

The *computational cost* of the first-last pivoting strategy is at most $2n - 2$ subtractions and $4n - 4$ multiplications. In Theorem 3.4 of [9] it was shown that Gaussian elimination with first-last pivoting can always be applied to transform a nonsingular sign-regular matrix into an upper triangular matrix.

As observed in Remark 3.5 of [9], it is easy to see that for a nonsingular sign-regular matrix the first-last pivoting strategy does not produce row exchanges if and only if either A or $-A$ is totally positive. Totally positive matrices are matrices with all their minors nonnegative. When A is totally positive, the backward stability of GE without row exchanges had been proved in [3]. Totally positive matrices arise naturally in many areas of mathematics, statistics and economics.



If A is a nonsingular sign-regular matrix, let P be the permutation matrix associated with the first-last pivoting strategy and let $B := PA$. By Corollary 3.5 of [9], B admits an LU -decomposition such that (2) holds. So, as commented above, we can conclude that the growth factors $\rho_n^W(A)$ and $\rho_n(A)$ are minimal (i.e., their value is 1).

The following result collects some basic information about the first-last pivoting strategy. We shall use that, if we assume that a matrix B is nonsingular and that no row exchanges are needed when performing GE then it is well known that one has, for $i \geq t, j \geq t$,

$$b_{ij}^{(t)} = \frac{\det B[1, 2, \dots, t-1, i | 1, 2, \dots, t-1, j]}{\det B[1, 2, \dots, t-1]}. \quad (3)$$

Proposition 7. *Let A be a nonsingular sign-regular matrix such that we perform GE with the first-last pivoting strategy. If LU is the triangular decomposition associated to this pivoting strategy then*

$$\frac{\| |L| |U| \|_\infty}{\|A\|_\infty} = 1, \quad (4)$$

the matrices $\tilde{A}^{(t)} = (\tilde{a}_{ij}^{(t)})_{1 \leq i, j \leq n}$ of (1) satisfy for each $t = 1, \dots, n$

$$\frac{|\tilde{a}_{tj}^{(t)}|}{|\tilde{a}_{tt}^{(t)}|} \leq \frac{|\tilde{a}_{ij}^{(t)}|}{|\tilde{a}_{it}^{(t)}|} \quad (5)$$

for all $i, j \in \{t, t+1, \dots, n\}$ and the matrices $A^{(t)}[t, \dots, n]$ are sign-regular for all t .

Proof. Let P be the permutation matrix associated with the first-last pivoting strategy and let $B := PA$. By Corollary 3.5 of [9], B admits an LU -decomposition such that

$$|B| = |L| |U|. \quad (6)$$

and (4) follows.

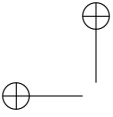
Observe that the first t rows of $B^{(t)}$ coincide with the first t rows of $A^{(t)}$ and that the remaining rows coincide up to permutation. Therefore, in order to prove the result, it is sufficient to see that

$$\frac{|b_{tj}^{(t)}|}{|b_{tt}^{(t)}|} \leq \frac{|b_{ij}^{(t)}|}{|b_{it}^{(t)}|} \quad (7)$$

for all $i, j \in \{t, t+1, \dots, n\}$. By (6) we can derive

$$|L[t, \dots, n]| |U[t, \dots, n]| = |L[t, \dots, n]U[t, \dots, n]| = |B^{(t)}[t, \dots, n]|. \quad (8)$$

Let us denote $\bar{B} := |B^{(t)}[t, \dots, n]|$, $\bar{L} := |L[t, \dots, n]|$ and $\bar{U} := |U[t, \dots, n]|$. Then (8) provides the LU -decomposition of $\bar{B} = (\bar{b}_{ij})_{1 \leq i, j \leq n-t+1}$. Observe that $\bar{b}_{ij} =$



$b_{i+t-1, j+t-1}^{(t)}$. We can write

$$\bar{B}^{(2)}[2, \dots, n-t+1] = \bar{L}[2, \dots, n-t+1]\bar{U}[2, \dots, n-t+1] \geq 0. \quad (9)$$

By (3) we derive for all $i, j \geq t$

$$0 \leq \bar{b}_{i-t+1, j-t+1}^{(2)} = \frac{\det \bar{B}[1, i-t+1|1, j-t+1]}{\bar{b}_{11}} = \frac{\det B^{(t)}[t, i|t, j]}{|b_{tt}^{(t)}|}$$

and so

$$0 \leq |b_{ij}^{(t)}| - \frac{|b_{tj}^{(t)}||b_{it}^{(t)}|}{|b_{tt}^{(t)}|}$$

and then (7) holds. Finally, the matrices $A^{(t)}[t, \dots, n]$ are sign-regular by Theorem 3.4 of [9]. \square

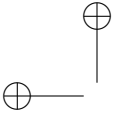
Let us now interpret (5) with respect to $\text{Cond}(U)$. As shown in p. 155 of [5], ill-conditioning in the sense of Skeel of the triangular matrix U must come from the fact that its rows have off-diagonal elements which are large relative to the diagonal element. Formula (5) ensures that, at each step of GE with the first-last pivoting, we choose as pivot row the row whose off-diagonal elements are smallest relative to diagonal elements. Therefore the first-last pivoting leads to an upper triangular matrix with Skeel condition number as small as possible.

If A is the inverse of an $n \times n$ sign-regular matrix and J_n is the diagonal matrix $J_n := \text{diag}\{1, -1, 1, \dots, (-1)^{n-1}\}$ then by formula (1.32) of [2] the matrix $J_n A J_n$ is sign-regular. Then, by Proposition 4.3 of [9], the solution x of $Ax = b$ is of the form $J_n y$, where y is the solution of the sign-regular linear system $J_n A J_n y = J_n b$. Therefore, in order to perform GE of A , we can carry out GE with first-last pivoting to $J_n A J_n$.

A nonsingular matrix A is an M -matrix if it has positive diagonal entries, non-positive off-diagonal entries and A^{-1} is nonnegative. M -matrices have very important applications, for instance, in iterative methods in numerical analysis, in the analysis of dynamical systems, in economics and in mathematical programming. The following pivoting strategies were introduced in [10].

Let A be a nonsingular $n \times n$ matrix. A row (resp., symmetric) pivoting strategy which chooses as pivot at the t th step ($t = 1, \dots, n-1$) of Gaussian elimination a row i_t satisfying $|a_{i_t t}^{(t)}| \geq \sum_{j>t} |a_{i_t j}^{(t)}|$ (resp., $|a_{i_t i_t}^{(t)}| \geq \sum_{j \geq t, j \neq i_t} |a_{i_t j}^{(t)}|$) whenever possible is called a row (resp., symmetric) diagonal dominance (d.d.) pivoting strategy. There are two main examples of row and symmetric d.d. pivoting strategies, depending on considering either maximal relative or maximal absolute diagonal dominance. A row (resp., symmetric) *maximal relative diagonal dominance* (m.r.d.d.) pivoting is a pivoting (resp., symmetric pivoting) which chooses as pivot at the t th step ($1 \leq t \leq n-1$) a row i_t satisfying

$$\frac{|a_{i_t t}^{(t)}|}{\sum_{j>t} |a_{i_t j}^{(t)}|} = \max_{t \leq i \leq n} \left\{ \frac{|a_{it}^{(t)}|}{\sum_{j>t} |a_{ij}^{(t)}|} \right\}$$



(resp.,

$$\frac{|a_{i_t i_t}^{(t)}|}{\sum_{j \geq t, j \neq i_t} |a_{i_t j}^{(t)}|} = \max_{t \leq i \leq n} \left\{ \frac{|a_{ii}^{(t)}|}{\sum_{j \geq t, j \neq i} |a_{ij}^{(t)}|} \right\}.$$

By Proposition 4.5 of [10], the symmetric m.r.d.d. pivoting strategy coincides with the symmetric scaled partial pivoting strategy for $\|\cdot\|_1$. A row (resp., symmetric) maximal absolute diagonal dominance (m.a.d.d.) pivoting is a row (resp., symmetric) pivoting which chooses as pivot at the t th step ($1 \leq t \leq n-1$) a row i_t satisfying

$$|a_{i_t i_t}^{(t)}| - \sum_{j > t} |a_{i_t j}^{(t)}| = \max_{t \leq i \leq n} \left\{ |a_{ii}^{(t)}| - \sum_{j > t} |a_{ij}^{(t)}| \right\}$$

(resp.,

$$|a_{i_t i_t}^{(t)}| - \sum_{j \geq t, j \neq i_t} |a_{i_t j}^{(t)}| = \max_{t \leq i \leq n} \left\{ |a_{ii}^{(t)}| - \sum_{j \geq t, j \neq i} |a_{ij}^{(t)}| \right\}.$$

Taking into account the well-known fact that into account that the Schur complement of a nonsingular M -matrix is also an M -matrix, we may deduce that, if A is a nonsingular M -matrix and we perform GE with any symmetric pivoting strategy, then all matrices $A^{(t)}$ of (1) are also M -matrices.

As shown in Remark 4.6 and Proposition 4.7 of [10], if A is a nonsingular $n \times n$ M -matrix, the symmetric m.a.d.d. pivoting strategy consists of choosing as pivot row in each step the row whose elements give a maximal sum and it adds $\mathcal{O}(n^2)$ elementary operations to the computational cost of the complete Gaussian elimination. In fact, following the notations of Proposition 4.7 of [10], let $e := (1, \dots, 1)^T$ and $b_1 := Ae$. The symmetric m.a.d.d. pivoting strategy produces the sequence of matrices (1) and the corresponding sequence of vectors:

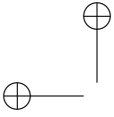
$$b_1 = b_1^{(1)} \longrightarrow \tilde{b}_1^{(1)} \longrightarrow b_1^{(2)} \longrightarrow \tilde{b}_1^{(2)} \longrightarrow \dots \longrightarrow b_1^{(n)} = \tilde{b}_1^{(n)} = c.$$

Then, as shown in Proposition 4.7 of [10], the largest component of $b_1^{(k)}[k, \dots, n]$ determines the k th pivot of m.a.d.d.

Given a nonsingular M -matrix A and any symmetric d.d. pivoting strategy, we obtained in Theorem 2.1 of [11] that $\rho_n(A) = 1$ and $\kappa(U) \leq \kappa(A)$. If A is a nonsingular M -matrix, then it is known (see, for instance, the proof of Theorem 4.4 of [10]) that any symmetric d.d. pivoting strategy leads to an upper triangular matrix U which is strictly diagonally dominant by rows. In this case, by Proposition 5,

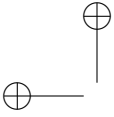
$$\text{Cond}(U) \leq (1/(2p-1)),$$

which is a bound independent of n .



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