A Comparison of Pivoting Strategies for the Direct LU Factorization

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Abstract

We combine the idea of the direct LU factorization with the idea of the pivoting strategy in the usual Gaussian elimination and show that t-wo so-called total scaled and total pivoting strategies can be employed in addition to the traditional pivoting strategies: partial scaled, partial, and direct diagonal. In this paper we offer a general LU factorization with total scaled pivoting algorithm from which the other well-known pivoting and non-pivoting algorithms can be driven. We utilize the random number routines in MSU-Billings' main frame computer to compare these pivoting strategies and conclude that none of the five strategies is absolutely more accurate than the other but generally their accuracy desending order is the same as their appearing order in the above.

1. Introduction

Let n and m be positive integers. Let A be an n by n matrix of real or complex numbers. Let B be an n by m matrix. To solve the linear system:

$$AX = B$$

many pivoting strategies have been developed for A being of some special type. One who is interested may refer to recent articles, for example, [1] and [2]. In this paper we shall be concerned with the case when A is of the general type. It is well known that by using Gaussian elimination with one of the following pivoting strategies: partial, partial scaled, and total one

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can solve the system by the backward substitution. It is also well known that if A can be LU factorized, one can solve the system with the forward substitution corresponding to the matrix L followed by the backward substitution corresponding to the matrix U. Recall that A can be directly LU factorized whenever the Gaussian elimination can be employed without any pivoting strategy, i.e., without row or column interchanges. Thus in order to solve the system one may use different strategies to find the LU factorization factors of A and at the same time permute the rows of the matrix X or the rows of the matrix B according to whether a pair of columns or rows of A are interchanged. After the LU factorization of A are found, the forward substitution and the backward substitutions can be applied and finally the rows of X are permuted back to its original order. In this paper we use these principles to combine the direct LU factorization with various pivoting strategies. In Section 2 we give some mathematical facts. The four pivoting strategies: partial, partial scaled, total, and total scaled are discussed in Section 3. Althought the direct Gaussian elimination method is omited in our discussion because it is strait forward, we compare it with the other in program. A general algorithm is given in Section 4. Then the other well-known pivoting and non-pivoting algorithms are driven from the general algorithm. In the last section we give a report on the accuracy among these stategies. The result is surprising that in 100000 random cases, even the simplest direct diagonal strategy is more accurate than the other in 8457 cases. These shows that none of the five strategies is absolutely more accurate than the other. We may conclude that generally speaking, the accuracy of the five pivoting strategies from the total scaled pivoting strategy to the direct diagonal pivoting strategy is descending.

2. Mathematical Discussion

(2.1) Notation. Let $I_n^{(i,j)}$ and $I_{n(i,j)}$ be the matrix induced from the n by n identity matrix by interchanging the ith and the jth rows and columns respectively.

(2.2) Notation. Let P be an n by m matrix. Let $P^{(i,j)}$ denote the matrix induced by interchanging the ith row and the jth row of P . Let $P_{(s,t)}$ denote the matrix induced by interchanging the sth column and the

tth column of P. Thus $P^{(s,t)}_{(i,j)}$ denotes the matrix induced by interchanging the ith and the jth row followed by interchanging the sth and the tth column or vice versa.

(2.3) Lemma. Let P be an n by m matrix. Then we have

$$P^{(i,j)} = I_n^{(i,j)} P$$

and

$$P_{(s,t)} = P I_{m(s,t)},$$

where, $1 \leq i, j \leq n$ and $1 \leq s, t \leq m$.

Proof. It is trivial from the definition of the matrix multiplication.

(2.4) Corollary. Let P be an n by m matrix. Then we have

$$P^{(i,j)}_{(s,t)} = I_n^{(i,j)} P I_{m(s,t)},$$

where, $1 \leq i, j \leq n$ and $1 \leq s, t \leq m$.

Proof. This an immediate consequence of the above lemma.

(2.5) Discussion, Definition and Notation. Let

$$\{F_i(\alpha, \beta) = 0\}_{i=1}^{n}$$

be a set of constraints. Let A be an n by n matrix. We say that A can be LU factorized up to the ith stage with respect to the constraints $\{F_i(\alpha, \beta) = 0\}_{i=1}^{n}$ if the following system of conditions:

$$F_j(l_{jj}, u_{jj}) = 0, \tag{A}$$

where $1 \leq j \leq i$, has a solution such that

$$l_{jj} u_{jj} \neq 0, \tag{B}$$

for $1 \leq j \leq i$, and

$$l_{jr} = 0, \tag{C}$$

where $1 \leq j \leq i, j < r \leq n$, and

$$u_{rt} = 0, \tag{D}$$

where $1 \leq t \leq i, t < r \leq n$, and

$$\sum_{r=1}^{min\{j,t\}} l_{jr} u_{rt} = a_{jt}, \tag{E}$$

where j and t are not simultaneously greater than i. Let L be a matrix with these solved entries l_{jr}, and U be a matrix with these solved entries u_{rt}. Then LU and A have the same entries except the right lower $(n-i)$ by $(n-i)$ entries. We write $A = LU/i/$.

In the rest of the paper, every matrix will be n by n and I will be the intentity matrix.

(2.6) Theorem. Let $\{F_i(\alpha,\beta) = 0\}_{i=1}^n$ be as in (2.5). Assume that A can be LU factorized up to the ith stage with respect to the given constraints such that $A = LU/i/$. Let $i < k, h, v, w \leq n$. Then $A_{(h,w)}^{(k,v)}$ which is the matrix induced from A by interchanging the kth and hth rows also the vth and the wth columns can be LU factorized up to the ith stage. Moreover we have $A_{(h,w)}^{(k,v)} = L^{(k,v)} U_{(h,w)}/i/$.

Proof. From Corollary (2.4) and Lemma (2.3) we have

$$A_{(h,w)}^{(k,v)} = I^{(k,v)} A I_{(h,w)}$$

and

$$I^{(k,v)} LU I_{(h,w)} = L^{(k,v)} U_{(h,w)}.$$

Since $L^{(k,v)}$ is induced from L by interchanging the kth and the vth rows and $U_{(h,w)}$ is induced from U by interchanging the hth and the wth columns and every index is greater than i conditions (A) - (E) of (2.5) are preserved. Therefore we obtain

$$A_{(h,w)}^{(k,v)} = L^{(k,v)} U_{(h,w)}/i/,$$

i.e., $A^{(k,v)}_{(h,w)}$ can be LU factorized up to the ith stage.

(2.7) Theorem. Let F, A, L, U be as in (2.5). Assume that A can be factorized up to the $(i-1)$th stage so that $A = LU/i-1/$. Assume further that

(I) $c_i = a_{ii} - \sum_{r=1}^{i-1} l_{ir}u_{ri} \neq 0$

and that the simultaneous equations

(II) $F_i(\alpha,\beta) = 0$ and $\alpha\beta = c_i$

have a solution (α_{ii},β_{ii}).

Then A can be LU factorized up to the ith stage:

$$A = L'U'/i/,$$

where

(i) L' and L have the same entries in their first $i-1$ columns and rows; So are U' and U;

(ii) $l'_{ii} = \alpha_{ii}$; $u'_{ii} = \beta_{ii}$;

(iii) $l'_{ir} = 0$; $u'_{ri} = 0$; for $i < r \leq n$;

(iv) $l'_{ji} = \frac{a_{ji} - \sum_{r=1}^{i-1} l_{jr}u_{ri}}{u'_{ii}} = \frac{a_{ji} - \sum_{r=1}^{i-1} l'_{jr}u'_{ri}}{u'_{ii}}$ for $i < j \leq n$;

(v) $u'_{ij} = \frac{a_{ij} - \sum_{r=1} i-1 l_{ir}u_{rj}}{l'_{ii}} = \frac{a_{ij} - \sum_{r=1} i-1 l'_{ir}u'_{rj}}{l'_{ii}}$ for $i < j \leq n$.

Proof. Condition (I) and condition (II) implies that $\alpha_{ii} \neq 0$ and $\beta_{ii} \neq 0$ so that $l'_{ii} \neq 0$ and $u'_{ii} \neq 0$. Hence condition (A) and condition (B) in (2.5) are satisfied and the constructions of these entries in (iv) and (v) are meaningful. Therfore condition (iv) and condition (v) guarantees that condition (E) in (2.5) is satisfied also. Condition (C) and condition (D) of (2.5) are satisfied because of (iii).

3. Pivoting Strategies

To do LU factorization of A we first set $i = 1$ and $A^{(i-1)} = A$. Assume that $A^{(i-1)}$ is can be factorized up to $(i-1)$th stage. Use a certain pivoting stratege to select a pivoting element $a^{(i-1)}_{vw}$ in $A^{(i-1)}$. Now apply Theorem (2.6) we next swap $a^{(i-1)}_{ii}$ with $a^{(i-1)}_{vw}$ by interchanging corresponding rows and columns. Then apply Theorem (2.7) to factorize the induced matrix $A^{(i)}$ so that $A^{(i)}$ can be factorized up to ith stage. Thus we have various choices for the LU factorization factors $L^{(i)}$ and $U^{(i)}$ of $A^{(i)}$ because of various different pivoting elements. The first three pivoting strategies in the following make use of the idea in the traditional Gaussian elimination.

(3.1) Partial Pivoting. When $A^{(i)}$, $1 \le i \le n$, is induced from $A^{(i-1)}$ by selecting an entry $a_{jk}^{(i-1)}$ such that
(I) $i \le j \le n; \quad k = i;$
(II) $|a_{jk}^{(i-1)}| = max_{r=i}^{n} |a_{rk}^{(i-1)}|$,
the pivoting strategy is called partial.

(3.2) Partial Scaled Pivoting. When the condition (I) in (3.1) is reserved and the condition (II) is replaced by
(II') $|a_{jk}^{(i-1)}| = max_{r=i}^{n} \frac{|a_{rk}^{(i-1)}|}{max_{s=1}^{n} |a_{rs}^{(i-1)}|}$,
the pivoting strategy is called partial scaled.

(3.3) Total Pivoting. When the condition (I) and (II) in (3.1) are replaced by
(I") $i \le j, k \le n;$
(II") $|a_{jk}^{(i-1)}| = max_{r,s=i}^{n} |a_{rs}^{(i-1)}|$,
the pivoting strategy is called total.

(3.4) Total Scaled Pivoting. When the condition (I") in (3.3) is reserved and (II") is replace by
(II"') $|a_{jk}^{(i-1)}| = max_{r,s=i}^{n} \frac{|a_{rs}^{(i-1)}|}{max_{s=1}^{n} |a_{rs}^{(i-1)}|}$,
the pivoting strategy is called total scaled.

4. General Algorithm

In the first subsection we give a general algorithm. Then simplyfy it to special cases in subsection (4.2) to (4.4). Moreover in subsection (4.5) some well-known non-pivoting strategies are considered as very special cases of the general algorithm. Based on the discussions in Section 2 and 3, for a given set of constraints $\{F_i(\alpha,\beta)=0\}_{i=1}^{n}$, in order to solve the linear system $AX=B$ the matrix A is induced from $A^{(0)}=A$ to $A^{(n)}$ so that $L^{(i)}$ and $U^{(i)}$, $1\le i\le n$, are obtained correspondingly. At the same time the rows of B or the rows of X are interchanged accordingly. In practice we do not actually interchange them each time. Instead we use two index arrays to keep their updated order. This technique will save computer's interchanging time. Then make use of these two arrays to interchange the rows of X and B respectively. Let Y and C denote their final interchanged forms so that we have $A^{(n)}Y=C$, i.e., $L^{(n)}U^{(n)}Y=C$. Let Z be the solution of $L^{(n)}Z=C$. Then Y is the solutuion of $U^{(n)}Y=Z$. Finally make use the index array for the row order of X to restore Y back to X . In the following we will use L and U to represent these $L^{(i)}$ and $U^{(i)}$, $1\le i\le n$. The two index arrays mentioned in the above are denoted by XI and BI. The absolute maximum of each row in X will be stored in the array MAX.

(4.1) General LU Factorization With Total Scaled Pivoting Algorithm. To solve the linear system $AX=B$:

(1) Declare A, L, and U as two dimensional n by n arrays of complex numbers;

(2) Declare X, Y, Z, B, and C as two dimensional n by m arrays of complex numbers;

(3) Declare XI and BI, as one dimensional arrays (with length n) of integers;

(4) Declare MAX as an one dimensional array (with length n) of real numbers;

(5) Input the entries of A and B;

(6) Initialize XI and BI so that $XI_i=BI_i=i$, $1\le i\le n$;

(7) For i from 1 to n find the absolute maximum for the ith row of X, i.e., $MAX_i=max_{j=1}^{n}|a_{ij}|$;

(8) If $MAX_i=0$ then output no unique solution message and stop

(9) For i from 1 to n find a pivoting element a_{jk} so that $i\le j,k\le n$, and $\frac{|a_{jk}|}{MAX_j}=max_{r,s=i}^{n}\frac{|a_{rs}|}{MAX_r}$

(10) If $i<j$ then (a) interchange the ith and jth rows of A only for those entries from the ith column to the nth column ; (b) interchange BI_i and BI_j ; (c) interchange the ith and jth rows of L only for

those entries from the first column to the $(i-1)$th column; (d) interchange MAX_i and MAX_j;

(11) If $i < k$ then (a) interchange the ith and kth columns of A only for those entries from the ith row to the nth row; (b) interchange XI_i and XI_k; (c) interchange the ith and kth columns of U only for those entries from the first row to the $(i-1)$th row;

(12) If $a_{ii} - \sum_{r=1}^{i-1} l_{ir}u_{ri} = 0$, then output no unique solution message and stop;

(13) Find a solution (l_{ii}, u_{ii}) to the simultaneous equations $F_i(\alpha, \beta) = 0$ and $\alpha\beta = a_{ii} - \sum_{r=1}^{i-1} l_{ir}u_{ri}$;

(14) If $i < n$, then for j from $i+1$ to n

(15) Find the jth entry of the ith column of L as follows: $l_{ji} = \frac{a_{ji} - \sum_{r=1}^{i-1} l_{jr}u_{ri}}{u_{ii}}$

(16) Find the jth entry of the ith row of U as follows: $u_{ij} = \frac{a_{ij} - \sum_{r=1}^{i-1} l_{ir}u_{rj}}{l_{ii}}$;

(17) Transform B to its final form C: $c_{ij} = b_{BI_{ij}}$, $1 \leq i, j \leq n$;

(18) Use forward substitution to solve the linear system $LZ = C$: For j from 1 to n do for i from 1 to n do set $z_{ij} = \frac{c_{ij} - \sum_{r=1}^{i-1} l_{ir}z_{ri}}{l_{ii}}$;

(19) Use backward substitution to solve the linear system $UY = Z$: For t from 1 to n do for s from n downto 1 do set $y_{st} = \frac{z_{st} - \sum_{r=s+1}^{n} u_{sr}y_{rt}}{u_{ss}}$;

(20) Restore X back to its original order from Y: For i from 1 to n do for j from 1 to n do set $x_{XI_{ij}} = y_{ij}$;

(21) Output X;

(22) Stop.

(Note that when $i = 1$ the sum in (12), (15), (16), (18) is defined as 0 and so is the sum in (19) when $s = n$.)

(4.2) Total Pivoting Algorithm. One can obtain this from (4.1) by deleting (4.1.4), (4.1.7), (4.1.8), and (4.1.10.c); in (4.1.9) deleting MAX and adding the statement "If $a_{jk} = 0$, then output no unique solution and stop".

(4.3) Partial Scaled Pivoting Algorithm. This can be achieved from (4.1) by deleting Y in (4.1.2) XI in (4.1.3) and (4.1.6); k and s being fixed as i in (4.1.9); replacing Y by X in (4.1.19); deleting (4.1.11) and (4.1.20).

(4.4) Partial Pivoting Algorithm. This can be obtained by deleting Y in (4.1.2); deleting XI in (4.1.3) and (4.1.6); deleting (4.1.4), (4.1.10.d), (4.1.11), and (4.1.20); in (4.1.9) fixing k and s as i, deleting MAX, and adding the statement "If $a_{jk} = 0$, then output no unique solution and stop"; replacing Y by X in (4.1.19).

(4.5) Some Special Cases of Non-Pivoting Strategy. If no pivoting strategies are employed in (4.1), i.e., (4.1.3) - (4.1.4), (4.1.6) - (4.1.11), (4.1.17), (4.1.20) are deleted and replace C by B in (4.1.18) Y by X in (4.1.19) and delete Y in (4.1.2), the no-pivoting algorithm is called Doolittle's method when $\{F_i(\alpha,\beta) = \alpha - 1\}_{i=1}^{n}$; Crout's method when $\{F_i(\alpha,\beta) = \beta - 1\}_{i=1}^{n}$; Choleski's method when $\{F_i(\alpha,\beta) = \alpha - \beta\}_{i=1}^{n}$.

5. Implementation and Accuracy Comparison

(5.1) An implementation. A Pascal (a program, a sample run of the program, and 4 modules which actually provide more other features) implementation of the above algorithms has been run in the main frame VAX 8650 with VAX/VMX version 5.5 of Montana State University - Billings. There we declare all the matrices to have open dimension length. We also employ the random routines in the system to compare the accuracy of the above pivoting strategies. Note the program is in the file chen_ictcm8_pgm.pas and its sample run result is in the file chen_ictcm8_pgm.out. The four modules are in chen_ictcm8_luf.pas, chen_ictcm8_lup.pas, chen_ictcm8_sar.pas, and chen_ictcm8_sub.pas respectively.

(5.2) Accuracy Comparison. We find out that, usually, the accuracy desending order of these pivoting strategies is the same order as their appearing order in the Section 4: For exmple, in a program run to solve a set of randomly selected linear systems of 5 variables we obtain the following reults:

(I) In 10 random cases:

There are 4 cases in which the total scaled strategy is the most accurate;
There are 4 cases in which the total strategy is the most accurate;
There are 2 case in which the partial scaled strategy is the most accurate;
There are 3 cases in which the partial strategy is the most accurate;
There are 0 cases in which without pivoting strategy is the most accurate.

(II) In 100 random cases:

There are 44 cases in which the total scaled strategy is the most accurate;
There are 29 cases in which the total strategy is the most accurate;
There are 26 case in which the partial scaled strategy is the most accurate;
There are 26 cases in which the partial strategy is the most accurate;
There are 0 cases in which without pivoting strategy is the most accurate.

(III) In 1000 random cases:

There are 365 cases in which the total scaled strategy is the most accurate;
There are 330 cases in which the total strategy is the most accurate;
There are 265 case in which the partial scaled strategy is the most accurate;
There are 261 cases in which the partial strategy is the most accurate;
There are 0 cases in which without pivoting strategy is the most accurate.

(IV) In 10000 random cases:

There are 3395 cases in which the total scaled strategy is the most accurate;
There are 3211 cases in which the total strategy is the most accurate;
There are 2655 case in which the partial scaled strategy is the most accurate;
There are 2560 cases in which the partial strategy is the most accurate;
There are 144 cases in which without pivoting strategy is the most accurate.

(V) In 100000 random cases:

There are 30132 cases in which the total scaled strategy is the most accurate;

There are 29828 cases in which the total strategy is the most accurate;
There are 26103 case in which the partial scaled strategy is the most accurate;
There are 25028 cases in which the partial strategy is the most accurate;
There are 8457 cases in which without pivoting strategy is the most accurate.

(Note that in some special cases two or more different pivoting strategies may yield the same degree of errors, i.e., they are of the same degree accurate therefore they could be the most accurate. This is the reason why the total sum of each individual subcases is not exactly the same as the total cases (usually more than).)

(5,3) Conclusion. From the above result, we may conclude that: (1) Strictly speaking, none of the five strategies is absolutely more accurate than the other four strategies. (2) Generally speaking, the accuracy for the five strategies from the total scaled strategy to the direct strategy is in descending order.

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