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Simultaneous computation of the row and column rank profiles

Jean-Guillaume Dumas^{*‡}, Clément Pernet^{†‡} and Ziad Sultan^{*†‡}

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Abstract

Gaussian elimination with full pivoting generates a PLUQ matrix decomposition. Depending on the strategy used in the search for pivots, the permutation matrices can reveal some information about the row or the column rank profiles of the matrix. We propose a new pivoting strategy that makes it possible to recover at the same time both row and column rank profiles of the input matrix and of any of its leading sub-matrices. We propose a rank-sensitive and quad-recursive algorithm that computes the latter PLUQ triangular decomposition of an $m \times n$ matrix of rank r in $O(mnr^{\omega-2})$ field operations, with ω the exponent of matrix multiplication. Compared to the LEU decomposition by Malashonock, sharing a similar recursive structure, its time complexity is rank sensitive and has a lower leading constant. Over a word size finite field, this algorithm also improves the practical efficiency of previously known implementations.

1 Introduction

Triangular matrix decomposition is a fundamental building block in computational linear algebra. It is used to solve linear systems, compute the rank, the determinant, the nullspace or the row and column rank profiles of a matrix. The LU decomposition, defined for matrices whose leading principal minors are all nonsingular, can be generalized to arbitrary dimensions and ranks by introducing pivoting on sides, leading e.g. to the LQUP decomposition of [6] or the PLUQ decomposition [5, 8]. Many algorithmic variants exist allowing fraction free computations [8], in-place computations [2, 7] or sub-cubic rank-sensitive time complexity [11, 7]. More precisely, the pivoting strategy reflected by the permutation matrices P and Q is the key difference between these PLUQ decompositions.

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In numerical linear algebra [5], pivoting is used to ensure a good numerical stability, good data locality, and reduce the fill-in. In the context of exact linear algebra, the role of pivoting differs. Indeed, only certain pivoting strategies for these decompositions will reveal the rank profile of the matrix. The latter is crucial in many applications using exact Gaussian elimination, such as Gröbner basis computations [4] and computational number theory [10].

The *row rank profile* of an $m \times n$ matrix with rank r is a lexicographically smallest sequence of r row indices such that the corresponding rows of the matrix are linearly independent. Similarly the *column rank profile* is a lexicographically smallest sequence of r column indices such that the corresponding rows of the matrix are linearly independent.

The common strategy to compute the row rank profile is to search for pivots in a row-major fashion: exploring the current row, then moving to the next row only if the current row is zero. Such a PLUQ decomposition can be transformed into a CUP decomposition (where $C = PL$ is in column echelon form) and the first r values of the permutation associated to P are exactly the row rank profile [7]. A block recursive algorithm can be derived from this scheme by splitting the row dimension [6]. Similarly, the column rank profile can be obtained in a column major search: exploring the current column, and moving to the next column only if the current one is zero. The PLUQ decomposition can be transformed into a PLE decomposition (where $E = UQ$ is in row echelon form) and the first r values of Q are exactly the column rank profile [7]. The corresponding block recursive algorithm uses a splitting of the column dimension.

Recursive elimination algorithms splitting both row and column dimensions include the TURBO algorithm [3] and the LEU decomposition [9]. No connection is made to the computation of the rank profiles in any of them. The TURBO algorithm does not compute the lower triangular matrix L and performs five recursive calls. It therefore implies an arithmetic overhead compared to classic Gaussian elimination. The LEU decomposition aims at reducing the amount of permutations and therefore also uses many additional matrix products. As a consequence its time complexity is not rank-sensitive.

We propose here a pivoting strategy following a Z-curve structure and working on an incrementally growing leading sub-matrix. This strategy is first used in a recursive algorithm splitting both rows and columns which recovers simultaneously both row and column rank profiles. Moreover, the row and column rank profiles of any leading sub-matrix can be deduced from the P and Q permutations. We show that the arithmetic cost of this algorithm remains rank sensitive of the form $O(mnr^{\omega-2})$ where ω is the exponent of matrix multiplication. The best currently known upper bound for ω is 2.3727 [12]. As for the CUP and PLE decompositions, this PLUQ decomposition can be computed in-place. We also propose an iterative variant, to be used as a base-case.

Compared to the CUP and PLE decompositions, this new algorithm has the following new salient features:

- it computes *simultaneously* both rank profiles at the cost of one,
- it preserves the squareness of the matrix passed to the recursive calls,

thus allowing more efficient use of the matrix multiplication building block,

- it reduces the number of modular reductions in a finite field,
- a CUP and a PLE decompositions can be obtained from it, with row and column permutations only.

Compared to the LEU decomposition,

- it is in-place,
- its time complexity bound is rank sensitive and has a better leading constant,
- a LEU decomposition can be obtained from it, with row and column permutations.

In Section 2 we present the new block recursive algorithm. Section 3 shows the connection with the LEU decomposition and section 4 states the main property about rank profiles. We then analyze the complexity of the new algorithm in terms of arithmetic operations: first we prove that it is rank sensitive in Section 5 and second we show in section 6 that, over a finite field, it reduces the number of modular reductions when compared to state of the art techniques. We then propose an iterative variant in Section 7 to be used as a base-case to terminate the recursion before the dimensions get too small. Experiments comparing computation time and cache efficiency are presented in section 8.

2 A recursive PLUQ algorithm

We first recall the name of the main sub-routines being used: **MM** stands for matrix multiplication, **TRSM** for triangular system solving with matrix unknown (left and right variants are implicitly indicated by the parameter list), **PermC** for matrix column permutation, **PermR** for matrix row permutation, etc. For instance, we will use:

MM(C, A, B) to denote $C \leftarrow C - AB$,

TRSM(U, B) for $B \leftarrow U^{-1}B$ with U upper triangular,

TRSM(B, L) for $B \leftarrow BL^{-1}$ with L lower triangular.

We also denote by $T_{k,l}$ the transposition of indices k and l and by $L \setminus U$, the storage of the two triangular matrices L and U one above the other. Further details on these subroutines and notations can be found in [7]. In block decompositions, we allow for zero dimensions. By convention, the product of any $m \times 0$ matrix by an $0 \times n$ matrix is the $m \times n$ zero matrix.

We now present the block recursive algorithm 1, computing a PLUQ decomposition.

Algorithm 1 PLUQ

Input: $A = (a_{ij})$ a $m \times n$ matrix over a field

Output: P, Q : $m \times m$ and $n \times n$ permutation matrices

Output: r : the rank of A

Output: $A \leftarrow \begin{bmatrix} L \setminus U & V \\ M & 0 \end{bmatrix}$ where L is $r \times r$ unit lower triangular, U is $r \times r$ upper triangular, and

$$A = P \begin{bmatrix} L \\ M \end{bmatrix} [U \ V] Q.$$

if $m=1$ **then**

if $A = [0 \ \dots \ 0]$ **then** $P \leftarrow [1], Q \leftarrow I_n, r \leftarrow 0$

else

$i \leftarrow$ the col. index of the first non zero elt. of A

$P \leftarrow [1]; Q \leftarrow T_{1,i}, r \leftarrow 1$

 Swap $a_{1,i}$ and $a_{1,1}$

end if

Return (P, Q, r, A)

end if

if $n=1$ **then**

if $A = [0 \ \dots \ 0]^T$ **then** $P \leftarrow I_m; Q \leftarrow [1], r \leftarrow 0$

else

$i \leftarrow$ the row index of the first non zero elt. of A

$P \leftarrow [1], Q \leftarrow T_{1,i}, r \leftarrow 1$

 Swap $a_{i,1}$ and $a_{1,1}$

for $j = i + 1 \dots m$ **do** $a_{j,1} \leftarrow a_{j,1} a_{1,1}^{-1}$

end for

end if

Return (P, Q, r, A)

end if

▷ the trailing parts of the algorithm are shown on next pages

It is based on a splitting of the matrix in four quadrants. A first recursive call is done on the upper left quadrant followed by a series of updates. Then two recursive calls can be made on the anti-diagonal quadrants if the first quadrant exposed some rank deficiency. After a last series of updates, a fourth recursive call is done on the bottom right quadrant. Figure 1 illustrates the position of the blocks computed in the course of algorithm 1, before and after the final permutation with matrices S and T .

This framework differs from the one in [3] by the order in which the quadrants are treated, leading to only four recursive calls in this case instead of five in [3]. We will show in section 4 that this fact together with the special form of the block permutations S and T makes it possible to recover rank profile information. The correctness of algorithm 1 is proven in appendix A.

Remark 1. Algorithm 1 is in-place (as defined in [7, Definition 1]): all

$$\triangleright \text{Splitting } A = \begin{bmatrix} A_1 & A_2 \\ A_3 & A_4 \end{bmatrix} \text{ where } A_1 \text{ is } \lfloor \frac{m}{2} \rfloor \times \lfloor \frac{n}{2} \rfloor.$$

$$\text{Decompose } A_1 = P_1 \begin{bmatrix} L_1 \\ M_1 \end{bmatrix} [U_1 \ V_1] Q_1 \quad \triangleright \text{PLUQ}(A_1)$$

$$\begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \leftarrow P_1^T A_2 \quad \triangleright \text{PermR}(A_2, P_1^T)$$

$$\begin{bmatrix} C_1 & C_2 \end{bmatrix} \leftarrow A_3 Q_1^T \quad \triangleright \text{PermC}(A_3, Q_1^T)$$

$$\text{Here } A = \left[\begin{array}{cc|c} L_1 \setminus U_1 & V_1 & B_1 \\ M_1 & 0 & B_2 \\ \hline C_1 & C_2 & A_4 \end{array} \right].$$

$$D \leftarrow L_1^{-1} B_1 \quad \triangleright \text{TRSM}(L_1, B_1)$$

$$E \leftarrow C_1 U_1^{-1} \quad \triangleright \text{TRSM}(C_1, U_1)$$

$$F \leftarrow B_2 - M_1 D \quad \triangleright \text{MM}(B_2, M_1, D)$$

$$G \leftarrow C_2 - E V_1 \quad \triangleright \text{MM}(C_2, E, V_1)$$

$$H \leftarrow A_4 - E D \quad \triangleright \text{MM}(A_4, E, D)$$

$$\text{Here } A = \left[\begin{array}{cc|c} L_1 \setminus U_1 & V_1 & D \\ M_1 & 0 & F \\ \hline E & G & H \end{array} \right].$$

$$\text{Decompose } F = P_2 \begin{bmatrix} L_2 \\ M_2 \end{bmatrix} [U_2 \ V_2] Q_2 \quad \triangleright \text{PLUQ}(F)$$

$$\text{Decompose } G = P_3 \begin{bmatrix} L_3 \\ M_3 \end{bmatrix} [U_3 \ V_3] Q_3 \quad \triangleright \text{PLUQ}(G)$$

$$\begin{bmatrix} H_1 & H_2 \\ H_3 & H_4 \end{bmatrix} \leftarrow P_3^T H Q_2^T \quad \triangleright \text{PermR}(H, P_3^T); \text{PermC}(H, Q_2^T)$$

$$\begin{bmatrix} E_1 \\ E_2 \end{bmatrix} \leftarrow P_3^T E \quad \triangleright \text{PermR}(E, P_3^T)$$

$$\begin{bmatrix} M_{11} \\ M_{12} \end{bmatrix} \leftarrow P_2^T M_1 \quad \triangleright \text{PermR}(M_1, P_2^T)$$

$$\begin{bmatrix} D_1 & D_2 \end{bmatrix} \leftarrow D Q_2^T \quad \triangleright \text{PermR}(D, Q_2^T)$$

$$\begin{bmatrix} V_{11} & V_{12} \end{bmatrix} \leftarrow V_1 Q_3^T \quad \triangleright \text{PermR}(V_1, Q_3^T)$$

$$\text{Here } A = \left[\begin{array}{ccc|cc} L_1 \setminus U_1 & V_{11} & V_{12} & D_1 & D_2 \\ M_{11} & 0 & 0 & L_2 \setminus U_2 & V_2 \\ M_{12} & 0 & 0 & M_2 & 0 \\ \hline E_1 & L_3 \setminus U_3 & V_3 & H_1 & H_2 \\ E_2 & M_3 & 0 & H_3 & H_4 \end{array} \right].$$

$$\begin{aligned} I &\leftarrow H_1 U_2^{-1} && \triangleright \text{TRSM}(H_1, U_2) \\ J &\leftarrow L_3^{-1} I && \triangleright \text{TRSM}(L_3, I) \\ K &\leftarrow H_3 U_2^{-1} && \triangleright \text{TRSM}(H_3, U_2) \\ N &\leftarrow L_3^{-1} H_2 && \triangleright \text{TRSM}(L_3, H_2) \\ O &\leftarrow N - J V_2 && \triangleright \text{MM}(N, J, V_2) \\ R &\leftarrow H_4 - K V_2 - M_3 O && \triangleright \text{MM}(H_4, K, V_2); \text{MM}(H_4, M_3, O) \end{aligned}$$

$$\text{Decompose } R = P_4 \begin{bmatrix} L_4 \\ M_4 \end{bmatrix} [U_4 \ V_4] Q_4 \quad \triangleright \text{PLUQ}(R)$$

$$\begin{bmatrix} E_{21} & M_{31} & 0 & K_1 \\ E_{22} & M_{32} & 0 & K_2 \end{bmatrix} \leftarrow P_4^T [E_2 \ M_3 \ 0 \ K] \quad \triangleright \text{PermR}$$

$$\begin{bmatrix} D_{21} & D_{22} \\ V_{21} & V_{22} \\ 0 & 0 \\ O_1 & O_2 \end{bmatrix} \leftarrow \begin{bmatrix} D_2 \\ V_2 \\ 0 \\ O \end{bmatrix} Q_4^T \quad \triangleright \text{PermC}$$

$$\text{Here } A = \left[\begin{array}{ccc|ccc} L_1 \setminus U_1 & V_{11} & V_{12} & D_1 & D_{21} & D_{22} \\ M_{11} & 0 & 0 & L_2 \setminus U_2 & V_{21} & V_{22} \\ M_{12} & 0 & 0 & M_2 & 0 & 0 \\ \hline E_1 & L_3 \setminus U_3 & V_3 & I & O_1 & O_2 \\ E_{21} & M_{31} & 0 & K_1 & L_4 \setminus U_4 & V_4 \\ E_{22} & M_{32} & 0 & K_2 & M_4 & 0 \end{array} \right].$$

$$S \leftarrow \begin{bmatrix} I_{r_1+r_2} & & & & & \\ & I_{k-r_1-r_2} & & & & \\ & & I_{r_3+r_4} & & & \\ & & & & I_{m-k-r_3-r_4} & \\ & & & & & \\ I_{r_1} & & & & & \\ & I_{r_3} & & & & \\ & & & I_{r_2} & & \\ & & & & & I_{r_4} \\ & & & & & & I_{k-r_1-r_3} \\ & & & & & & & I_{n-k-r_2-r_4} \end{bmatrix}$$

$$P \leftarrow \text{Diag}(P_1 \begin{bmatrix} I_{r_1} \\ P_2 \end{bmatrix}, P_3 \begin{bmatrix} I_{r_3} \\ P_4 \end{bmatrix}) S$$

$$Q \leftarrow T \text{Diag}(\begin{bmatrix} I_{r_1} \\ Q_3 \end{bmatrix} Q_1, \begin{bmatrix} I_{r_2} \\ Q_4 \end{bmatrix} Q_2)$$

$$A \leftarrow S^T A T^T \quad \triangleright \text{PermR}(A, S^T); \text{PermC}(A, T^T)$$

$$\text{Here } A = \left[\begin{array}{ccc|cc} L_1 \setminus U_1 & D_1 & V_{11} & D_{21} & V_{12} & D_{22} \\ M_{11} & L_2 \setminus U_2 & 0 & V_{21} & 0 & V_{22} \\ E_1 & I & L_3 \setminus U_3 & O_1 & V_3 & O_2 \\ E_{21} & K_1 & M_{31} & L_4 \setminus U_4 & 0 & V_4 \\ M_{12} & M_2 & 0 & 0 & 0 & 0 \\ E_{22} & K_2 & M_{32} & M_4 & 0 & 0 \end{array} \right]$$

Return $(P, Q, r_1 + r_2 + r_3 + r_4, A)$

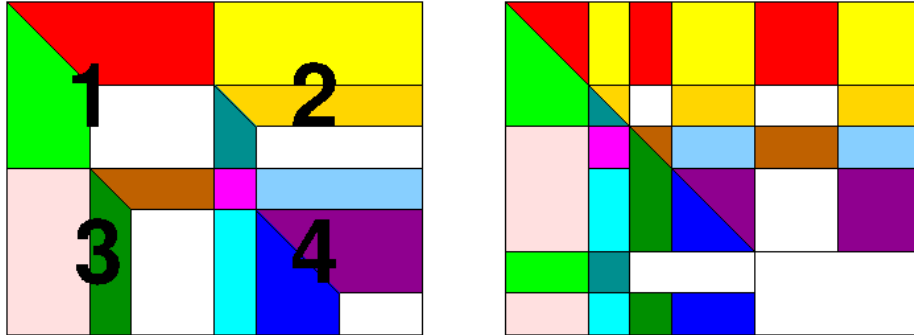


Figure 1: Block recursive Z-curve PLUQ decomposition and final block permutation.

operations of the *TRSM*, *MM*, *PermC*, *PermR* subroutines work with $O(1)$ extra memory allocations except possibly in the course of fast matrix multiplications. The only constraint is for the computation of $J \leftarrow L_3^{-1}I$ which would overwrite the matrix I that should be kept for the final output. Hence a copy of I has to be stored for the computation of J . The matrix I has dimension $r_3 \times r_2$ and can be stored transposed in the zero block of the upper left quadrant (of dimension $(\frac{m}{2} - r_1) \times (\frac{n}{2} - r_1)$, as shown on Figure 1).

3 From PLUQ to LEU

We now show how to compute the LEU decomposition of [9] from the PLUQ decomposition. The idea is to write

$$P \begin{bmatrix} L \\ M \end{bmatrix} [UV] Q = \underbrace{P \begin{bmatrix} L & 0 \\ M & I_{m-r} \end{bmatrix} P^T}_{\bar{L}} \underbrace{P \begin{bmatrix} I_r \\ 0 \end{bmatrix} Q}_{E} \underbrace{Q^T \begin{bmatrix} U & V \\ & I_{n-r} \end{bmatrix} Q}_{\bar{U}}$$

and show that \bar{L} and \bar{U} are respectively lower and upper triangular. This is not true in general, but turns out to be satisfied by the P, L, M, U, V and Q obtained in algorithm 1.

Theorem 1. *Let $A = P \begin{bmatrix} L \\ M \end{bmatrix} [UV] Q$ be the PLUQ decomposition computed by algorithm 1. Then for any unit lower triangular matrix Y and any upper triangular matrix Z , the matrix $P \begin{bmatrix} L \\ MY \end{bmatrix} P^T$ is unit lower triangular and $Q^T \begin{bmatrix} UV \\ Z \end{bmatrix} Q$ is upper triangular.*

Proof. Proceeding by induction, we assume that the theorem is true on all four recursive calls, and show that it is true for the matrices $P \begin{bmatrix} L \\ MY \end{bmatrix} P^T$ and $Q^T \begin{bmatrix} UV \\ Z \end{bmatrix} Q$. Let $Y = \begin{bmatrix} Y_1 \\ Y_2 Y_3 \end{bmatrix}$ where Y_1 is unit lower triangular of

dimension $k - r_1 - r_2$. From the correctness of algorithm 1 (see e.g.

$$\text{Equation A), } S \begin{bmatrix} L \\ MY \end{bmatrix} S^T = \begin{bmatrix} L_1 \\ M_{11} L_2 \\ M_{12} M_2 Y_1 \\ \hline E_1 \quad I \quad L_3 \\ E_{21} K_1 \quad M_{31} L_4 \\ E_{22} K_2 Y_2 M_{32} M_4 Y_3 \end{bmatrix}$$

Hence $P \begin{bmatrix} L \\ MY \end{bmatrix} P^T$ equals

$$\begin{bmatrix} P_1 \\ P_3 \end{bmatrix} \begin{bmatrix} I_{r_1} & & & \\ & P_2 & & \\ & & I_{r_3} & \\ & & & P_4 \end{bmatrix} \begin{bmatrix} L_1 \\ M_{11} L_2 \\ M_{12} M_2 Y_1 \\ \hline E_1 \quad I \quad L_3 \\ E_{21} K_1 \quad M_{31} L_4 \\ E_{22} K_2 Y_2 M_{32} M_4 Y_3 \end{bmatrix} \times \\ \begin{bmatrix} I_{r_1} & & & \\ & P_2^T & & \\ & & I_{r_3} & \\ & & & P_4^T \end{bmatrix} \begin{bmatrix} P_1^T \\ P_3^T \end{bmatrix}$$

By induction hypothesis, the matrices $\overline{L_2} = P_2 \begin{bmatrix} L_2 \\ M_2 Y_1 \end{bmatrix} P_2^T$, $\overline{L_4} = P_4 \begin{bmatrix} L_4 \\ M_4 Y_3 \end{bmatrix} P_4^T$

, $P_1 \begin{bmatrix} L_1 \\ M_1 \overline{L_2} \end{bmatrix} P_1^T$ and $P_3 \begin{bmatrix} L_3 \\ M_3 \overline{L_4} \end{bmatrix} P_3^T$ are unit lower triangular. Therefore the matrix $P \begin{bmatrix} L \\ MY \end{bmatrix} P^T$ is also unit lower triangular.

Similarly, let $Z = \begin{bmatrix} Z_1 Z_2 \\ Z_3 \end{bmatrix}$ where Z_1 is upper triangular of dimension $k - r_1 - r_2$. The matrix $T^T \begin{bmatrix} UV \\ Z \end{bmatrix} T$ equals

$$T^T \begin{bmatrix} U_1 V_{11} V_{12} & D_1 D_{21} D_{22} \\ 0 & 0 & U_2 V_{21} V_{22} \\ U_3 V_3 & 0 & O_1 O_2 \\ 0 & & U_4 V_4 \\ Z_1 & & Z_2 \\ & & Z_3 \end{bmatrix} = \begin{bmatrix} U_1 V_{11} V_{12} & D_1 D_{21} D_{22} \\ U_3 V_3 & O_1 O_2 \\ Z_1 & Z_2 \\ 0 & 0 & U_2 V_{21} V_{22} \\ 0 & & U_4 V_4 \\ & & Z_3 \end{bmatrix}$$

Hence $Q^T \begin{bmatrix} UV \\ Z \end{bmatrix} Q$ equals

$$\begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} \begin{bmatrix} I_{r_1} & & & \\ & Q_3^T & & \\ & & I_{r_2} & \\ & & & Q_4^T \end{bmatrix} \begin{bmatrix} U_1 V_{11} V_{12} & D_1 D_{21} D_{22} \\ U_3 V_3 & O_1 O_2 \\ Z_1 & Z_2 \\ 0 & 0 & U_2 V_{21} V_{22} \\ 0 & & U_4 V_4 \\ & & Z_3 \end{bmatrix} \times \\ \begin{bmatrix} I_{r_1} & & & \\ & Q_3 & & \\ & & I_{r_2} & \\ & & & Q_4 \end{bmatrix} \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}.$$

By induction hypothesis, the matrices $\bar{U}_3 = Q_3^T \begin{bmatrix} U_3 V_3 \\ Z_1 \end{bmatrix} Q_3$, $\bar{U}_4 = Q_4^T \begin{bmatrix} U_4 V_4 \\ Z_3 \end{bmatrix} P_4^T$, $Q_1^T \begin{bmatrix} U_1 V_1 \\ \bar{U}_3 \end{bmatrix} Q_1$ and $Q_2^T \begin{bmatrix} U_2 V_2 \\ \bar{U}_4 \end{bmatrix} Q_2$ are upper triangular. Consequently the matrix $Q^T \begin{bmatrix} U & V \\ Z \end{bmatrix} Q$ is upper triangular.

For the base case with $m = 1$. The matrix \bar{L} has dimension 1×1 and is unit lower triangular. If $r = 0$, then $\bar{U} = I_n^T Z I_n$ is upper triangular. If $r = 1$, then $Q = T_{1,i}$ where i is the column index of the pivot and is therefore the column index of the leading coefficient of the row $[UV] Q$. Applying Q^T on the left only swaps rows 1 and i , hence row $[UV] Q$ is the i th row of $Q^T \begin{bmatrix} UV \\ Z \end{bmatrix} Q$. The latter is therefore upper triangular. The same reasoning can be applied to the case $n = 1$. \square

Corollary 1. Let $\bar{L} = P \begin{bmatrix} L \\ MI_{m-r} \end{bmatrix} P^T$, $E = P \begin{bmatrix} I_r \\ 0 \end{bmatrix} Q$ and $\bar{U} = Q^T \begin{bmatrix} UV \\ 0 \end{bmatrix} Q$. Then $A = \bar{L}E\bar{U}$ is a LEU decomposition of A .

Remark 2. The converse is not always possible: given $A = L, E, U$, there are several ways to choose the last $m - r$ columns of P and the last $n - r$ rows of Q . The LEU algorithm does not keep track of these parts of the permutations.

4 Computing the rank profiles

We prove here the main feature of the PLUQ decomposition computed by algorithm 1: it reveals the row and column rank profiles of all leading sub-matrices of the input matrix. We recall in Lemma 1 basic properties verified by the rank profiles.

Lemma 1. For any matrix,

1. the row rank profile is preserved by right multiplication with an invertible matrix and by left multiplication with an invertible upper triangular matrix.
2. the column rank profile is preserved by left multiplication with an invertible matrix and by right multiplication with an invertible lower triangular matrix.

Lemma 2. Let $A = PLUQ$ be the PLUQ decomposition computed by algorithm 1. Then the row (resp. column) rank profile of any leading (k, t) submatrix of A is the row (resp. column) rank profile of the leading (k, t) submatrix of $P \begin{bmatrix} I_r \\ 0 \end{bmatrix} Q$.

Proof. With the notations of corollary 1, we have:

$$A = P \begin{bmatrix} L \\ MI_{m-r} \end{bmatrix} \begin{bmatrix} I_r \\ 0 \end{bmatrix} \begin{bmatrix} U & V \\ & I_{n-r} \end{bmatrix} Q = \bar{L}P \begin{bmatrix} I_r \\ 0 \end{bmatrix} Q\bar{U}$$

Hence

$$[I_k 0] A \begin{bmatrix} I_t \\ 0 \end{bmatrix} = \bar{L}_1 [I_k 0] P \begin{bmatrix} I_r \\ 0 \end{bmatrix} Q\bar{U}_1,$$

where \overline{L}_1 is the $k \times k$ leading submatrix of \overline{L} (hence it is an invertible lower triangular matrix) and \overline{U}_1 is the $t \times t$ leading submatrix of \overline{U} (hence it is an invertible upper triangular matrix). Now, Lemma 1 implies that the rank profile of $\begin{bmatrix} I_k 0 \\ 0 \end{bmatrix} A \begin{bmatrix} I_t \\ 0 \end{bmatrix}$ is that of $\begin{bmatrix} I_k 0 \\ 0 \end{bmatrix} P \begin{bmatrix} I_r \\ 0 \end{bmatrix} Q \begin{bmatrix} I_t \\ 0 \end{bmatrix}$. \square

From this lemma we deduce how to compute the row and column rank profiles of any (k, t) leading submatrix and more particularly of the matrix A itself.

Corollary 2. *Let $A = PLUQ$ be the PLUQ decomposition of a $m \times n$ matrix computed by algorithm 1. The row (resp. column) rank profile of any (k, t) -leading submatrix of a A is the sorted sequence of the row (resp. column) indices of the non zero rows (resp. columns) in the matrix*

$$R = \begin{bmatrix} I_k 0 \\ 0 \end{bmatrix} P \begin{bmatrix} I_r \\ 0 \end{bmatrix} Q \begin{bmatrix} I_t \\ 0 \end{bmatrix}$$

Corollary 3. *The row (resp. column) rank profile of A is the sorted sequence of row (resp. column) indices of the non zero rows (resp. columns) of the first r columns of P (resp. first r rows of Q).*

5 Complexity analysis

We study here the time complexity of algorithm 1 by counting the number of field operations. For the sake of simplicity, we will assume here that the dimensions m and n are powers of two. The analysis can easily be extended to the general case for arbitrary m and n .

For $i = 1, 2, 3, 4$ we denote by T_i the cost of the i -th recursive call to PLUQ, on a $\frac{m}{2} \times \frac{n}{2}$ matrix of rank r_i . We also denote by $T_{\text{TRSM}}(m, n)$ the cost of a call TRSM on a rectangular matrix of dimensions $m \times n$, and by $T_{\text{MM}}(m, k, n)$ the cost of multiplying an $m \times k$ by an $k \times n$ matrix.

Theorem 2. *Algorithm 1, run on an $m \times n$ matrix of rank r , performs $O(mnr^{\omega-2})$ field operations.*

Proof. Let $T = T_{\text{PLUQ}}(m, n, r)$ be the cost of algorithm 1 run on a $m \times n$ matrix of rank r . From the complexities of the subroutines given, e.g.,

in [2] and the recursive calls in algorithm 1, we have:

$$\begin{aligned}
T &= T_1 + T_2 + T_3 + T_4 + T_{\text{TRSM}}(r_1, \frac{m}{2}) + T_{\text{TRSM}}(r_1, \frac{n}{2}) \\
&\quad + T_{\text{TRSM}}(r_2, \frac{m}{2}) + T_{\text{TRSM}}(r_3, \frac{n}{2}) + T_{\text{MM}}(\frac{m}{2} - r_1, r_1, \frac{n}{2}) \\
&\quad + T_{\text{MM}}(\frac{m}{2}, r_1, \frac{n}{2} - r_1) + T_{\text{MM}}(\frac{m}{2}, r_1, \frac{n}{2}) \\
&\quad + T_{\text{MM}}(r_3, r_2, \frac{n}{2} - r_2) + T_{\text{MM}}(\frac{m}{2} - r_3, r_2, \frac{n}{2} - r_2 - r_4) \\
&\quad + T_{\text{MM}}(\frac{m}{2} - r_3, r_3, \frac{n}{2} - r_2 - r_4) \\
&\leq T_1 + T_2 + T_3 + T_4 + K \left(\frac{m}{2} (r_1^{\omega-1} + r_2^{\omega-1}) + \frac{n}{2} (r_1^{\omega-1} \right. \\
&\quad \left. + r_3^{\omega-1}) + \frac{m}{2} \frac{n}{2} r_1^{\omega-2} + \frac{m}{2} \frac{n}{2} r_2^{\omega-2} + \frac{m}{2} \frac{n}{2} r_3^{\omega-2} \right) \\
&\leq T_1 + T_2 + T_3 + T_4 + K' mnr^{\omega-2}
\end{aligned}$$

for some constants K and K' (we recall that $a^{\omega-2} + b^{\omega-2} \leq 2^{3-\omega}(a + b)^{\omega-2}$ for $2 \leq \omega \leq 3$).

Let $C = \max\{\frac{K'}{1-2^{4-2\omega}}; 1\}$. Then we can prove by a simultaneous induction on m and n that $T \leq Cmnr^{\omega-2}$.

Indeed, if $(r = 1, m = 1, n \geq m)$ or $(r = 1, n = 1, m \geq n)$ then $T \leq m - 1 \leq Cmnr^{\omega-2}$. Now if it is true for $m = 2^j, n = 2^i$, then for $m = 2^{j+1}, n = 2^{i+1}$, we have

$$\begin{aligned}
T &\leq \frac{C}{4} mn(r_1^{\omega-2} + r_2^{\omega-2} + r_3^{\omega-2} + r_4^{\omega-2}) + K' mnr^{\omega-2} \\
&\leq \frac{C(2^{3-\omega})^2}{4} mnr^{\omega-2} + K' mnr^{\omega-2} \\
&\leq K' \frac{2^{4-2\omega}}{1-2^{4-2\omega}} mnr^{\omega-2} + K' mnr^{\omega-2} \leq Cmnr^{\omega-2}.
\end{aligned}$$

□

In order to compare this algorithm with usual Gaussian elimination algorithms, we now refine the analysis to compare the leading constant of the time complexity in the special case where the matrix is square and has a generic rank profile: $r_1 = \frac{m}{2} = \frac{n}{2}, r_2 = 0, r_3 = 0$ and $r_4 = \frac{m}{2} = \frac{n}{2}$ at each recursive step.

Hence we have

$$\begin{aligned}
T_{\text{PLUQ}} &= 2T_{\text{PLUQ}}(\frac{n}{2}, \frac{n}{2}, \frac{n}{2}) + 2T_{\text{TRSM}}(\frac{n}{2}, \frac{n}{2}) + T_{\text{MM}}(\frac{n}{2}, \frac{n}{2}, \frac{n}{2}) \\
&= 2T_{\text{PLUQ}}(\frac{n}{2}, \frac{n}{2}, \frac{n}{2}) + 2\frac{C_\omega}{2^{\omega-1}-2} \left(\frac{n}{2}\right)^\omega + C_\omega \left(\frac{n}{2}\right)^\omega
\end{aligned}$$

Writing $T_{\text{PLUQ}}(n, n, n) = \alpha n^\omega$, the constant α satisfies:

$$\alpha = C_\omega \frac{1}{(2^\omega - 2)} \left(\frac{1}{2^{\omega-2} - 1} + 1 \right) = C_\omega \frac{2^{\omega-2}}{(2^\omega - 2)(2^{\omega-2} - 1)}.$$

which is equal to the constant of the CUP and LUP decompositions [7, Table 1]. In particular, it equals $2/3$ when $\omega = 3, C_\omega = 2$, matching the constant of the classical Gaussian elimination.

6 Number of modular reductions over a prime field

In the following we suppose that the operations are done with full delayed reduction for a single multiplication and any number of additions: operations of the form $\sum a_i b_i$ are reduced only once at the end of the addition, but $a \cdot b \cdot c$ requires two reductions. In practice, only a limited amount of accumulations can be done on an actual mantissa without overflowing, but we neglect this in this section for the sake of simplicity. See e.g. [2] for more details. For instance, with this model, the number of reductions required by a classic multiplication of matrices of size $m \times k$ by $k \times n$ is simply: $m \cdot n$. We denote this by $R_{MM}(m, k, n) = mn$. This extends e.g. also for triangular solving:

Theorem 3. *Over a prime field modulo p , the number of reductions modulo p required by $TRSM(m, n)$ with full delayed reduction is:*

$$\begin{aligned} R_{UnitTRSM}(m, n) &= mn \quad \text{if the triangular matrix is unitary,} \\ R_{TRSM}(m, n) &= 2mn \quad \text{in general.} \end{aligned}$$

Proof. If the matrix is unitary, then a fully delayed reduction is required only once after the update of each row of the result. In the generic case, we invert each diagonal element first and multiply each element of the right hand side by this inverse diagonal element, prior to the update of each row of the result. This gives mn extra reductions. \square

Next we show that the new pivoting strategy is more efficient in terms of number of integer division.

Theorem 4. *Over a prime field modulo p and on a full-rank square $m \times m$ matrix with generic rank profile, and m a power of two, the number of reductions modulo p required by the elimination algorithms with full delayed reduction is:*

$$\begin{aligned} R_{PLUQ}(m, m) &= 2m^2 + o(m^2), \\ R_{PLE}(m, m) = R_{CUP}(m, m) &= (1 + \frac{1}{4} \log_2(m)) m^2 + o(m^2) \end{aligned}$$

Proof. If the top left square block is full rank then PLUQ reduces to one recursive call, two square TRSM (one unitary, one generic) one square matrix multiplication and a final recursive call. In terms of modular reductions, this gives: $R_{PLUQ}(m) = 2R_{PLUQ}(\frac{m}{2}) + R_{UnitTRSM}(\frac{m}{2}, \frac{m}{2}) + R_{TRSM}(\frac{m}{2}, \frac{m}{2}) + R_{MM}(\frac{m}{2}, \frac{m}{2}, \frac{m}{2})$. Therefore, using theorem 3, the number of reductions within PLUQ satisfies $T(m) = 2T(\frac{m}{2}) + m^2$ so that it is $R_{PLUQ}(m, m) = 2m^2 - 2m$ if m is a power of two.

For row or column oriented elimination this situation is more complicated since the recursive calls will always be rectangular even if the intermediate matrices are full-rank. We in fact prove, by induction on m , the more generic:

$$R_{PLE}(m, n) = \log_2(m) \left(\frac{mn}{2} - \frac{m^2}{4} \right) + m^2 + o(mn + m^2) \quad (1)$$

First $R_{PLE}(1, n) = 0$ since $[1] \times [a_1, \dots, a_n]$ is a triangular decomposition of the $1 \times n$ matrix $[a_1, \dots, a_n]$. Now suppose that Equation 1 holds

for $k = m$. Then we follow the row oriented algorithm of [2, Lemma 5.1] which makes two recursive calls, one TRSM and one MM to get $R_{\text{PLE}}(2m, n) = R_{\text{PLE}}(m, n) + R_{\text{PLE}}(m, m) + R_{\text{MM}}(m, m, n-m) + R_{\text{PLE}}(m, n-m) = R_{\text{PLE}}(m, n) + R_{\text{PLE}}(m, n-m) + m(n+m)$. We then apply the induction hypothesis on the recursive calls to get

$$\begin{aligned} R_{\text{PLE}}(2m, n) &= \frac{1}{2} \log_2(m)mn - \frac{1}{4} \log_2(m)m^2 + m^2 + \\ &\quad \frac{1}{2} \log_2(m)m(n-m) - \frac{1}{4} \log_2(m)m^2 + m^2 + \\ &\quad m(n+m) + o(mn+m^2) \\ &= \log_2(m)(mn - m^2) + 3m^2 + mn + o(mn+m^2). \end{aligned}$$

The latter is also obtained by substituting $k \leftrightarrow 2m$ in Equation 1 so that the induction is proven. \square

This show that the new algorithm requires much less modular reductions, as soon as m is larger than 32. Over finite fields, since reductions can be much more expensive than multiplications or additions by elements of the field, this is a non negligible advantage. We show in the next section that this participates to the better practical performance of the PLUQ algorithm.

7 A base case algorithm

We propose in algorithm 2 an iterative algorithm computing the same PLUQ decomposition as algorithm 1. The motivation is to offer an alternative to the recursive algorithm improving the computational efficiency on small matrix sizes. Indeed, as long as the matrix fits the cache memory, the amount of page faults of the two variants are similar, but the iterative algorithm reduces the amount of row and column permutations. The block recursive algorithm can then be modified so that it switches to the iterative algorithm whenever the matrix dimensions are below a certain threshold.

Unlike the common Gaussian elimination, where pivots are searched in the whole current row or column, the strategy is here to proceed with an incrementally growing leading sub-matrix. This implies a Z-curve type search scheme, as shown on figure 2. This search strategy is meant to ensure the properties on the rank profile that have been presented in section 4.

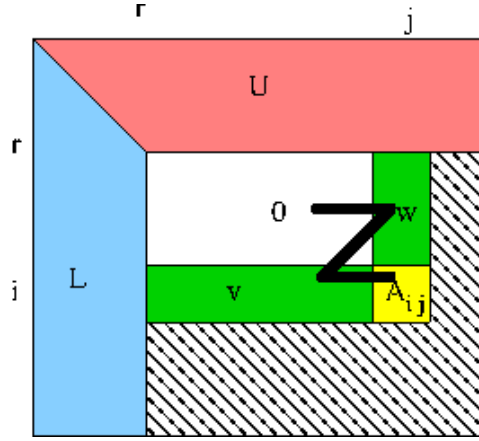


Figure 2: Iterative base case PLUQ decomposition

Algorithm 2 PLUQ iterative base case

Input: A a $m \times n$ matrix over a field

Output: P, Q : $m \times m$ and $n \times n$ permutation matrices

Output: r : the rank of A

Output: $A \leftarrow \begin{bmatrix} L & UV \\ M & 0 \end{bmatrix}$ where L is $r \times r$ unit lower triang., U is $r \times r$ upper

triang. and such that $A = P \begin{bmatrix} L \\ M \end{bmatrix} [UV] Q$.

$r \leftarrow 0; i \leftarrow 0; j \leftarrow 0$

while $i < m$ or $j < n$ **do**

\triangleright Let $v = [A_{i,r} \dots A_{i,j-1}]$ and $w = [A_{r,j} \dots A_{i-1,r}]^T$

if $j < n$ and $w \neq 0$ **then**

$p \leftarrow$ row index of the first non zero entry in w

$q \leftarrow j; j \leftarrow \max(j+1, n)$

else if $i < m$ and $v \neq 0$ **then**

$q \leftarrow$ column index of the first non zero entry in v

$p \leftarrow i; i \leftarrow \max(i+1, m)$

else if $i < m$ and $j < n$ and $A_{i,j} \neq 0$ **then**

$(p, q) \leftarrow (i, j)$

$i \leftarrow \max(i+1, m); j \leftarrow \max(j+1, n)$

else

$i \leftarrow \max(i+1, m); j \leftarrow \max(j+1, n)$

continue

end if

\triangleright At this stage, $A_{p,q}$ is a pivot

for $k = p+1 \dots n$ **do**

$A_{k,q} \leftarrow A_{k,p}/A_{p,q}$

$A_{k,q+1 \dots n} \leftarrow A_{k,q+1 \dots n} - A_{k,q}A_{p,q+1 \dots n}$

end for

$A_{r+1 \dots m, r+1} \leftrightarrow A_{r+1 \dots m, q}$

\triangleright Swap pivot column

$A_{r+1, r+1 \dots n} \leftrightarrow A_{p, r+1 \dots n}$

\triangleright Swap pivot row

$P \leftarrow T_{p,r}P; Q \leftarrow QT_{q,r}$

14

$\triangleright T_{k,l}$ swaps indices k and l

$r \leftarrow r+1$

end while

Remark 3. *In order to further improve the data locality, this iterative algorithm can be transformed into a left-looking variant [1]. We did not write this version here for the sake of clarity, but this is how we implemented the base case for the experiments of section 8.*

8 Experiments

We present here experiments comparing an implementation of algorithm 1 computing a PLUQ decomposition against the implementation of the CUP/PLE decomposition, called LUdivine in the FFLAS-FFPACK library¹. The new implementation of the PLUQ decomposition is available in this same library from version svn@346. We ran our tests on a single core of an Intel Xeon E5-4620@2.20GHz using gcc-4.7.2.

Figures 3 and 4 compare the computation time of LUdivine, and the new PLUQ algorithm. In figure 3, the matrices are dense, with full rank. The computation times are similar, the PLUQ algorithm with base case showing a slight improvement over LUdivine. In figures 4 and 5, the

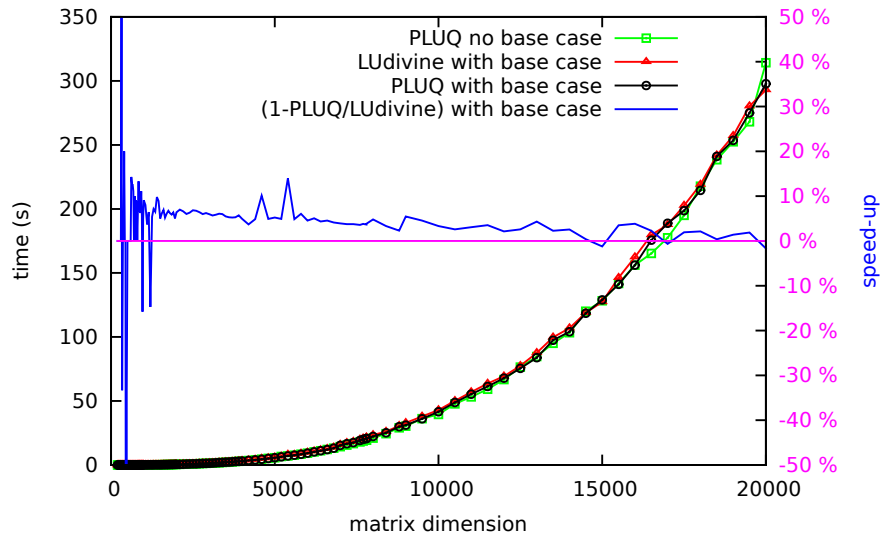


Figure 3: Computation time with dense full rank matrices over $\mathbb{Z}/1009\mathbb{Z}$.

matrices are square, dense with a rank equal to half the dimension. To ensure non trivial row and column rank profiles, they are generated from a LEU decomposition, where L and U are uniformly random non-singular lower and upper triangular matrices, and E is zero except on $r = n/2$ positions, chosen uniformly at random, set to one. The cutoff dimension for the switch to the base case has been set to an optimal value of 30 by experiments. Figure 4 shows how the base case greatly improves the efficiency for PLUQ, presumably for it reduces the number of row and column

¹<http://linalg.org/fflas-ffpack>

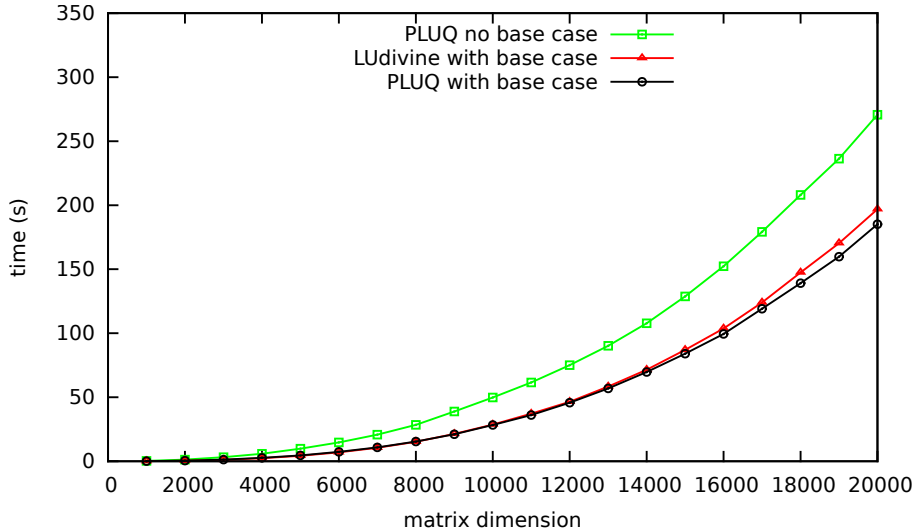


Figure 4: Computation time with dense rank deficient matrices (rank is half the dimension)

permutations. With the base case the computation time is comparable to LUdivine. More precisely, PLUQ becomes faster than LUdivine for dimensions above 9000. Figure 5 shows that, on larger matrices, PLUQ can be about 10% faster than LUdivine.

Table 1 summarizes some of the data reported by the callgrind tool of the valgrind emulator (version 3.8.1) concerning the cache misses. We also report in the last column the corresponding computation time on the machine (without emulator). The matrices used are the same as in figure 4, with rank half the dimension. We first notice the impact of the base case on the PLUQ algorithm: although it does not change the number of cache misses, it strongly reduces the total number of memory accesses (less permutations), thus improving the computation time. Now as the dimension grows, the total amount of memory accesses and the amount of cache misses plays in favor of PLUQ which becomes faster than LUdivine.

9 Conclusion and perspectives

The decomposition that we propose can first be viewed as an improvement over the LEU decomposition, introducing a finer treatment of rank deficiency that reduces the number of arithmetic operations, makes the time complexity rank sensitive and allows to perform the computation in-place.

Second, viewed as a variant of the existing CUP/PLE decompositions, this new algorithm produces more information on the rank profile and has

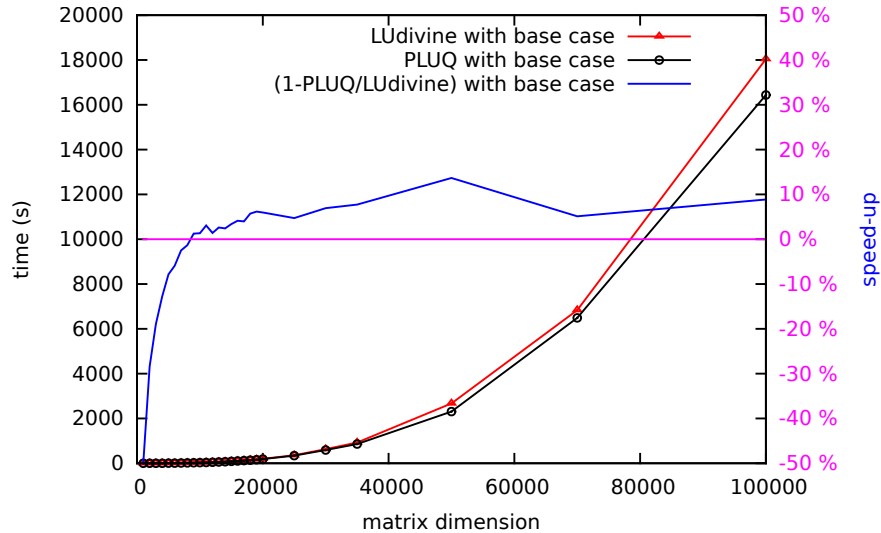


Figure 5: Computation time with dense rank deficient matrices of larger dimension

better cache efficiency, as it avoids calling matrix products with rectangular matrices of unbalanced dimensions. It also performs fewer modular reductions when computing over a finite field.

Overall the new algorithm is also faster in practice than previous implementations when matrix dimensions get large enough.

Now, in a parallel setting, it should exhibit more parallelism than row or column major eliminations since the recursive calls in step 2 and 3 are independent. This is also the case for the TURBO algorithm of [3], but the latter requires more arithmetic operations. Further experiments and analysis of communication costs have to be conducted in shared and distributed memory settings to assess the possible practical gains in parallel.

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Matrix	Algorithm	Accesses	L1 Misses	LL Misses	Relative	Timing (s)
A4K	PLUQ-no-base-case	1.319E+10	7.411E+08	1.523E+07	.115	5.84
	PLUQ-base-case	8.119E+09	7.414E+08	1.526E+07	.188	2.65
	LUdivine	1.529E+10	1.246E+09	2.435E+07	.159	2.35
A8K	PLUQ-no-base-case	6.150E+10	5.679E+09	1.305E+08	.212	28.4
	PLUQ-base-case	4.072E+10	5.681E+09	1.306E+08	.321	15.4
	LUdivine	7.555E+10	9.693E+09	2.205E+08	.292	15.2
A12K	PLUQ-no-base-case	1.575E+11	1.911E+10	4.691E+08	.298	75.1
	PLUQ-base-case	1.112E+11	1.911E+10	4.693E+08	.422	45.7
	LUdivine	2.003E+11	3.141E+10	7.943E+08	.396	46.4
A16K	PLUQ-no-base-case	3.142E+11	4.459E+10	1.092E+09	.347	152
	PLUQ-base-case	2.302E+11	4.459E+10	1.092E+09	.475	99.4
	LUdivine	4.117E+11	7.391E+10	1.863E+09	.452	103

Table 1: Cache misses for dense matrices with rank equal half of the dimension

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A Correctness of algorithm 1

First note that $S \begin{bmatrix} L \\ M \end{bmatrix} = \left[\begin{array}{c|c} L_1 & \\ \hline M_{11} L_2 & \\ M_{12} M_2 & 0 \\ \hline E_1 & I \quad L_3 \\ E_{21} K_1 M_{31} L_4 & \\ E_{22} K_2 M_{32} M_4 0 & \end{array} \right]$

Hence $P \begin{bmatrix} L \\ M \end{bmatrix} = \begin{bmatrix} P_1 & \\ & P_3 \end{bmatrix} \left[\begin{array}{c|c} L_1 & \\ \hline M_1 P_2 \begin{bmatrix} L_2 \\ M_2 \end{bmatrix} & \\ \hline E_1 & I \quad L_3 \\ E_2 & K \quad M_3 P_4 \begin{bmatrix} L_4 \\ M_4 \end{bmatrix} \end{array} \right]$

Similarly, $[UV]T = \left[\begin{array}{c|c} U_1 V_{11} V_{12} & D_1 D_{21} D_{22} \\ 0 & U_2 V_{21} V_{22} \\ U_3 V_3 & 0 \quad O_1 \quad O_2 \\ & U_4 \quad V_4 \\ & 0 \end{array} \right]$ and $[UV]Q = \left[\begin{array}{c|c} U_1 & V_1 & D_1 & D_2 \\ & 0 & U_2 & V_2 \\ [U_3 V_3] Q_3 & 0 & O & O \\ & [U_4 V_4] Q_4 & & \end{array} \right] \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$.

Now as $H_1 = IU_2, H_2 = IV_2 + L_3 O, H_3 = KU_2$ and $H_4 = KV_2 + M_3 O + P_4 \begin{bmatrix} L_4 \\ M_4 \end{bmatrix} [U_4 V_4] Q_4$ we have

$$\begin{aligned} P \begin{bmatrix} L \\ M \end{bmatrix} [UV]Q &= \begin{bmatrix} P_1 & \\ & P_3 \end{bmatrix} \left[\begin{array}{c|c} L_1 & \\ \hline M_1 P_2 \begin{bmatrix} L_2 \\ M_2 \end{bmatrix} & \\ \hline E_1 & I \quad L_3 \\ E_2 & K \quad M_3 P_4 \begin{bmatrix} L_4 \\ M_4 \end{bmatrix} \end{array} \right] \\ & \left[\begin{array}{c|c} U_1 & V_1 & D_1 & D_2 \\ & 0 & U_2 & V_2 \\ [U_3 V_3] Q_3 & 0 & O & O \\ & [U_4 V_4] Q_4 & & \end{array} \right] \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} \\ &= \begin{bmatrix} P_1 & \\ & P_3 \end{bmatrix} \left[\begin{array}{c|c} L_1 & \\ \hline M_1 P_2 \begin{bmatrix} L_2 \\ M_2 \end{bmatrix} & \\ \hline E_1 & I_{r_3} \\ E_2 & I_{m-k-r_3} \end{array} \right] \\ & \left[\begin{array}{c|c} U_1 & V_1 & D_1 D_2 \\ & 0 & U_2 V_2 \\ L_3 [U_3 V_3] Q_3 & H_1 H_2 \\ M_3 [U_3 V_3] Q_3 & H_3 H_4 \end{array} \right] \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} \\ &= \begin{bmatrix} P_1 & \\ & I_{m-k} \end{bmatrix} \left[\begin{array}{c|c} L_1 & \\ \hline M_1 & \\ \hline E & O I_{m-k} \end{array} \right] \begin{bmatrix} U_1 V_1 D \\ 0 & F \\ G & H \end{bmatrix} \\ & \begin{bmatrix} Q_1 \\ I_{n-k} \end{bmatrix} \\ &= \begin{bmatrix} P_1 & \\ & I_{m-k} \end{bmatrix} \left[\begin{array}{c|c} L_1 U_1 & L_1 V_1 & B_1 \\ M_1 U_1 & M_1 V_1 & B_2 \\ C_1 & C_2 & A_4 \end{array} \right] \begin{bmatrix} Q_1 \\ I_{n-k} \end{bmatrix} \\ &= A \end{aligned}$$