LU and Cholesky matrix factorization algorithms are core subroutines used to solve systems of linear equations (SLEs) encountered while solving an optimization problem. Standard factorization algorithms are highly efficient but remain susceptible to the accumulation roundoff errors, which can lead solvers to return feasibility and optimality certificates that are actually invalid. This paper introduces a novel approach for solving sequences of closely related SLEs encountered in nonlinear programming efficiently and without roundoff errors. Specifically, it introduces rank-one update algorithms for the roundoff-error-free (REF) factorization framework, a toolset built on integer-preserving arithmetic that has led to the development and implementation of fail-proof SLE solution subroutines for linear programming. The formal guarantees of the proposed algorithms are formally established through the derivation of theoretical insights. Their computational advantages are supported with computational experiments, which demonstrate upwards of 75x-improvements over exact factorization run-times on fully dense matrices with over one million entries.

A significant advantage of the proposed methodology is that the length of any coefficient calculated via the associated algorithms is bounded polynomially in the size of the inputs without having to resort to greatest common divisor operations, which are required by and thereby hinder an efficient implementation of exact rational arithmetic approaches.

**Key words:** Exact mathematical programming, nonlinear optimization, matrix factorizations, low-rank modifications

**History:** various sources

1. **Introduction**

LU and Cholesky matrix factorization algorithms are widely used in mathematical programming software to solve systems of linear equations (SLEs). They are long established in linear programming (LP), where the factorizations are utilized in the simplex algorithm to move between basic solutions efficiently through the application of factorization updates. They are similarly prevalent in mixed integer linear programming (MILP), where they are used within the branch-and-bound algorithm to efficiently solve LP relaxations of closely related subproblems (e.g., those of close successor nodes). For analogous reasons, LU and Cholesky matrix factorization algorithms are increasingly utilized in nonlinear programming and augmented intelligence.
programming (NLP), where they are deployed within a number of algorithms to solve sequences of SLEs, which are similar to one another but in ways that are substantially different from the LP/MILP setting. In NLP, the updates of interest are rank-one updates and downdates and, more generally, low-rank modifications of the constraint coefficient matrix. As a primary example, rank-one updates of LU and Cholesky factorizations are used to reflect iterative changes to the Hessian and Jacobian matrices associated with the solution of KKT systems of constrained NLPs (Stange et al. 2007). It is worth remarking that low-rank updates have been also prominently featured in LP interior point methods (e.g., see Mehrotra (1992), Pan (2020)).

Low-rank factorization updates are essential for the efficient deployment of various algorithms including fast model predictive control (MPC) (Herceg et al. 2015, Kirches et al. 2011), which are employed in the distillation of hazardous chemical compounds and other critical applications (Drgoňa et al. 2017). Rank-one updates of Cholesky factorizations are widely used in a variety of machine learning applications that incorporate linear models or kernels. They are used, for example, to quickly recompute the solution to least squares support vector machine (LS-SVM) classifier problems (Fine and Scheinberg 2001), which can be modeled as linearly constrained quadratic programs (Ojeda et al. 2008). They are also utilized to perform Bayesian inference via the expected propagation method (Seeger et al. 2007), which can be modeled as linearly constrained bilevel NLPs (Minka 2013).

Increased numerical stability is among the chief reasons that LU and Cholesky factorization algorithms are preferred over alternative approaches for solving sequences of closely related SLEs. For instance, the Sherman-Morrison-Woodbury (SWM) formula has been widely used (and continues to be, to a certain extent) to perform low-rank modifications of the inverse matrix efficiently (Seeger 2008). However, the implementation of the SWM formula is particularly vulnerable to compounding roundoff errors and their deleterious consequences. In fact, the benefits of replacing its use with low-rank factorization updates have been corroborated extensively (e.g., see Fine and Scheinberg (2001), Ojeda et al. (2008)). In spite of their relatively superior numerical stability, matrix factorization algorithms remain susceptible to the accumulation of roundoff errors inherent in floating point computations, which can affect the behavior of optimization solvers and the validity of their outputs. The types of incongruous outcomes that may occur—often unbeknownst to users—include, but are not limited to, optimal solutions being wrongly eliminated from the
feasible domain (Bailey and Borwein 2015), a problem being incorrectly identified as having no feasible solutions (Pan 2015, Puranik and Sahinidis 2017), and failing to converge to the optimal solution (Choi et al. 1990, Fine and Scheinberg 2001).

Although these and other invalid outcomes are admittedly infrequent, their non-negligible plausibility detracts from the implicit trust placed on mathematical programming software. Their potential occurrence is specially concerning when obtaining an invalid certificate of feasibility/infeasibility or optimality/suboptimality is exceedingly costly or intolerable (Magron et al. 2017, Sarra 2011). In optimal design applications, for instance, decisions must be taken based on very few observations. Therefore, inferences obtained via the solution of a sequence of linearly constrained NLPs, for which Cholesky factorization rank-one updates can be applied, must be both valid and highly accurate (Seeger et al. 2007). Similar concerns are germane to the real-time operation of adaptive systems, which are used to protect radio electronic systems (e.g., radar) by processing spatiotemporal signals on a “sliding-window” (Lekhovytskiy 2018).

This paper introduces a novel approach for performing fast and exact factorization updates, for the purpose of constructing fail-proof and efficient validation routines for nonlinear programming and other contexts where it is necessary to solve SLEs that undergo low-rank modifications. The featured approach is a direct solution method with various notable differences from existing factorization update algorithms. First, it is founded on specialized integer-preserving arithmetic subroutines, meaning that all operations performed within the featured algorithms—inclusive of division—are guaranteed to be exact. These subroutines make efficient use of unlimited-precision data types. In fact, the length of any coefficient they encounter is bounded polynomially in the size of the inputs without having to resort to greatest common divisor (GCD) operations, which are required by any comparable direct solution method approach built on exact rational arithmetic. Another distinctive feature of the proposed approach is that the updated factorization is not obtained by modifying the original factorization; instead, it is reconstructed through an iterative process that leverages fundamental links between the two factorizations derived herein. The introduction of this approach leads to three main contributions: (1) Derivation of new theoretical insights that help establish the correctness of the factorization update algorithms; (2) Efficient fail-proof algorithms for updating exact LU and Cholesky factorizations in $O(n^2)$ operations; and (3) A study to compare the computational performance of the proposed update algorithms and exact refactorization.
The article is organized as follows. Section 2 provides a background on LU and Cholesky factorizations and on the integer-preserving framework featured in the proposed approach. Section 3 derives the theoretical insights that serve as the foundation of the fast and exact rank-one algorithms, which are introduced in Section 4. Section 5 introduces a study on fully-dense matrices that demonstrates the computational benefits of the proposed algorithms. Finally, Section 6 concludes the article and discusses future research directions.

2. Background
Define an SLE $Ax = b$, with coefficient matrix $A \in \mathbb{Q}^{m \times n}$ of rank $m \leq n$, right-hand side parameter vector $b \in \mathbb{Q}^m$, and variable vector $x \in \mathbb{Q}^n$. An LU factorization of $A$ is defined as a pair of matrices $L$ and $U$, the former lower-triangular and the latter upper-triangular, such that $LU = A$. In general, the LU factorization of $A$ is not unique and its computation requires $O(n^3)$ operations. When $A$ is symmetric, it is possible to compute a (unique) factorization of the form $LL^T$ (a lower-triangular matrix, times its transpose) known as the Cholesky factorization. Once the respective factorization has been obtained, the SLE can be solved for any instantiation of $b$ through forward substitution and backward substitution, in $O(n^2)$ operations (fewer operations may be required when $A$ has a special structure). The first of these algorithm entails solving for $y \in \mathbb{Q}^n$ in the triangular system $Ly = b$, and the second algorithm entails solving for $x \in \mathbb{Q}^n$ in the triangular system $Ux = y$.

The remainder of this section is organized as follows. Section 2.1 provides a basic description of SLE rank-one and low-rank updates and one of their primary uses in NLP, and it reviews existing factorization-based algorithms. Section 2.2 describes the integer-preserving framework upon which the exact factorizations featured in this work are constructed. Lastly, Section 2.3 summarizes two approaches for performing LP-related updates on these factorizations, and it explains their inadequacy for performing rank-one updates.

2.1. Rank-one and Low-rank Factorization Updates
In mathematical programming and various other fields, it is often necessary to solve a sequence of closely related SLEs. That is, after solving the system $Ax = b$ via factorization (or another suitable method), one needs to solve the updated system $\hat{A}x = b'$, where $\hat{A} \in \mathbb{Q}^{m \times n}$ has full row-rank and is obtained from a relatively simple modification of $A$, and $b' \in \mathbb{Q}^n$ is an arbitrary right-hand side parameter vector. For certain modifications, it
is possible to obtain an LU factorization of $\hat{A}$ (i.e., $\hat{L}\hat{U}$) in $O(n^2)$ operations by updating an existing LU factorization of $A$. A rank-one update is one such modification given by:

$$\hat{A} = A + \gamma v w^T,$$

(1)

where $\gamma \in Q^1$, $v \in Q^m$, and $w \in Q^n$ s.t. $v \neq 0$ and $w \neq 0$ (i.e., the outer product $vw^T$ has rank one). In the closely related rank-one downdate, the matrix $\gamma vw^T$ is subtracted from $A$. In either case, a symmetry-preserving update can be performed when $v = w$ and $A$ is symmetric, which is relevant to the Cholesky factorization. Furthermore, Equation (1) can be generalized into a low-rank or rank-$k$ update by replacing vectors $v, w$ with matrices $V \in Q^{m \times k}$, $W \in Q^{n \times k}$, respectively, where $k \geq 1$ is usually much smaller than $m$.

Rank-one updates are core components of NLP algorithms. As a prominent example, the symmetric-rank-one (SR1) formula is used in Quasi-Newton methods to update an approximation matrix $B$ of the Hessian as

$$\hat{B} = B + \frac{(u - Bs)(u - Bs)^T}{(u - Bs)^T s},$$

where $u$ and $s$ are $n \times 1$ vectors and $B$ is an $n \times n$ matrix (see (Wright et al. 1999)). The SR1 formula is obtained from the symmetry-preserving rank-one update $A + \gamma vv^T$ (where $v \in Q^n$ in this case) by setting $A = B$, $v = u - Bs$, and $\gamma = 1/(u - Bs)^T s$. Moreover, the two-sided rank-one update formula (TR1) is used to update an approximation matrix $C$ of the Jacobian as

$$\hat{C} = C + \frac{(r - Cs)(\mu^T - \sigma^T C)}{\mu^T s - \sigma^T Cs},$$

where $r$ and $\sigma$ are $m \times 1$ vectors, $\mu$ is an $n \times 1$ vector, and $C$ is an $m \times n$ matrix, with $n \geq m$ (see (Griewank and Walther 2002)). The TR1 formula is obtained from Equation (1) by setting $A = C$, $v = r - Cs$, $w = (\mu^T - \sigma^T C)^T$, and $\gamma = 1/(\mu^T s - \sigma^T Cs)$. Matrices $B$ and $C$ are the coefficients of linearized KKT systems whose solution provides the next point and Lagrangian multipliers used in the optimization algorithm. Accordingly, these SLEs can be efficiently solved via LU factorization updates (Stange et al. 2007).

Various algorithms have been defined for performing low-rank updates efficiently, beginning with Bennett (1965) who introduced a rank-$k$ update algorithm for LDU factorizations—which consist of a lower-triangular, a diagonal, and an upper-triangular matrix factor—that iteratively changes matrices $L$ and $U$ by applying Gaussian
elimination-type operations (e.g., row reduction, matrix permutation). Fletcher and Powell (1974) developed a variant of this algorithm for the special case when $k = 1$, $U = L^T$, and $D$ is positive definite. Kielbasiński and Schwetlick (1988) introduced a related approach for performing rank-one updates on LU factorizations, which may encounter problems when $A$ is rectangular (Stange et al. 2007). Gill et al. (1974) describe various approaches for performing rank-one updates on Cholesky factorizations and one such algorithm for matrices that may not be symmetric positive definite. The best performing algorithms utilize plane rotation methods consisting of Householder transformations or products of Givens matrices. Such methods are also commonly utilized for QR factorizations—a decomposition of $A$ into an orthogonal and an upper trapezoidal matrix (Hammarling and Lucas 2008).

More recent works on factorization updates have focused on Cholesky factorization algorithms owing to their superior stability on positive-definite and quasi-definite coefficient matrices (Deng 2010, Gill et al. 1996, Higham 2009). In fact, Bennet’s algorithm is numerically stable only when $A$ and the rank-$k$ matrices are symmetric and $D$ is positive definite (Gill et al. 1974). Yet, the advantageous numerical properties of Cholesky factorization are guaranteed only under certain technical conditions (Gill et al. 1996), not to mention that numerous critical engineering applications deal with coefficient matrices that are neither quasi-definite nor symmetric—e.g., optimal power flow (Oh and Hu 2018). To deal with a broader class of matrices, Stange et al. (2007) introduced three LU update algorithms adapted from those of Bennett (1965), Fletcher and Matthews (1985), and Kielbasiński and Schwetlick (1988). These adaptations emphasize numerical stability by allowing different row/column permutations not defined in the original versions. Computational results therein demonstrate a superior performance of LU-based methods over QR-based methods including in their application to solve KKT systems of an NLP test set of Hock and Schittkowski (1980). However, they also demonstrate that both implementations still deviate from the expected theoretical convergence on quadratic optimization problems.

This work derives fail-proof algorithms for performing rank-one updates on exact matrix factorizations. The algorithms are applicable to LU and Cholesky factorizations and, unlike existing LU factorization algorithms, their efficacy does not depend on pivot strategies (Higham 2011) or parameter tuning (Stange et al. 2007). The featured algorithms are also applicable to rank-one downdates, which tend to cause problems when using floating-point arithmetic due to possible cancellations when the rank-one matrix is subtracted from $A$. 
To the best of our knowledge, this is the first work to develop a fast and exact direct solution approach for performing NLP-related factorization updates. The ensuing subsections introduce the exact arithmetic framework that serves as the foundation of the proposed approach.

2.2. The Roundoff-error-free Factorization Framework

The proposed theory and algorithms build on the roundoff-error-free (REF) factorization framework, a direct solution approach that utilizes exact integer-preserving arithmetic. The REF factorization framework includes subroutines for constructing exact LU and Cholesky factorizations and for solving SLEs exactly via REF forward and backward substitution, both for dense (Escobedo and Moreno-Centeno 2015) and sparse matrices (Lourenco et al. 2019). REF factorization subroutines are significantly faster than their exact rational arithmetic counterparts (Escobedo et al. 2018). In fact, the sparse variants of the REF framework represent the only known exact factorization algorithms for solving SLEs in time proportional to arithmetic work (Lourenco 2020). They are now included in MATLAB’s SuiteSparse libraries (Lourenco et al. 2020), through which they have been employed in real-world engineering applications—e.g., Diaz-Hernandez et al. (2021) used the REF framework to improve the accuracy and computational performance of large-scale models for harbor agitation climate assessment. Exact rational arithmetic factorization algorithms generally cannot solve SLEs in time proportional to arithmetic work because they must constantly carry out GCD operations to prevent exponential growth in the bit-length or encoding size of the matrix entries (Weber et al. 2019). Conversely, REF factorization algorithms achieve the former guarantee through a set of special properties derived from the integer-preserving Gaussian elimination algorithm (IPGE).

To establish a proper foundation for this work, the ensuing paragraphs introduce assumptions, notational conventions, IPGE, and the REF factorization algorithms.

**Assumption 1.** For the remainder of this work, let \( A \in \mathbb{Z}^{n \times n} \) and \( \hat{A} = A + \gamma v w^T \) be nonsingular, and assume that \( b, v, w \in \mathbb{Z}^n \) and \( \gamma \in \mathbb{Z}^1 \).

**Definition 1.** Let \([k]\) be shorthand for the ordered index set \(\{1, \ldots, k\}\), where \(k \geq 1\).

**Definition 2.** Denote \( A_{[k],j} \) as the submatrix induced by the ordered column-index set \(\{1, \ldots, k, j\}\) and the ordered row-index set \(\{1, \ldots, k, i\}\) of \(A\); similarly, denote \(v_{[k],i}\) as the subvector induced from \(v\) by the ordered index set \(\{1, \ldots, k, i\}\).
Definition 3. Let $A^{(k)}$ be the $k$th-iteration matrix of IPGE, for integer $0 \leq k \leq n$, where $A^{(0)} := A$. Denote the individual entries of this matrix as $a_{i,j}^{(k)}$, for $1 \leq i,j \leq n$.

Definition 4. Let the scalar $\rho^{(k)}$ denote the pivot element selected from $A^{(k-1)}$ to perform the $k$th iteration of IPGE, where $\rho^{(0)} := 1$.

Definition 5. The recursive formula for calculating IPGE entry $a_{i,j}^{(k)}$ is given by:

$$a_{i,j}^{(k)} = \begin{cases} a_{i,j}^{(k-1)} & \text{if } i = r_k \\ \rho^{(k)}a_{i,j}^{(k-1)} - a_{r_k,j}^{(k-1)}a_{i,c_k}^{(k-1)} / \rho^{(k-1)} & \text{otherwise} \end{cases}$$

for $k = 1 \ldots n$ (2)

where $1 \leq i, j, k \leq n$ and $\rho^{(k)} \neq 0$ for all $k$; and where $r_k$ and $c_k$ are the row and column indices, respectively, of $\rho^{(k)}$ in $A^{k-1}$.

Assumption 2. Fix $\rho^{(k)} = a_{k,k}^{(k-1)} \neq 0$ (i.e., $r_k = c_k = k$), for $k \geq 1$.

Prior to introducing the REF factorization algorithms, it is useful to elaborate on the preceding assumptions. Assumption 1 does not lead to a loss of generality since any rational matrix can be multiplied by the lowest common denominator of its entries and any finite-precision matrix can be multiplied (i.e., right-shifted) by an adequate power of 10 to yield an SLE whose coefficients are all integers. Assumption 2 implies that IPGE does not need to perform row/column permutations to find nonzero pivot elements and is adopted for simplicity. For extended algorithms that deal with the possibility of encountering zeros along the diagonal, see Escobedo (2016).

It is important also to highlight three properties ensured by IPGE. First, every division performed in the algorithm is guaranteed to be exact (Bareiss 1968), that is, each dividend is an integer multiple of its divisor. Second, the bit-length of any IPGE entry, denoted as $\beta_{\text{max}}$, is bounded polynomially as $\beta_{\text{max}} \leq \lceil n \log(\sigma \sqrt{n}) \rceil$, where $\sigma := \max_{i,j} |a_{i,j}^{(0)}|$ (Bareiss 1972). Third, each IPGE entry $a_{i,j}^{(k)}$ equates to a specific subdeterminant of $A$, as follows (Edmonds 1967):

$$a_{i,j}^{(k)} = \begin{cases} (-1)^{i+k} \det(A_{[k]\setminus i\cup j}^{[k]}) & \text{if } i \leq k \\ \det((A)_{[k]\setminus i,j}^{[k]}) & \text{otherwise}; \end{cases}$$

for $0 \leq k \leq n$ and $1 \leq i,j \leq n$. Based on this characterization, Assumption 2 implies that, for any $k \geq 1$, the subvectors $A_{[k]}^1, A_{[k]}^2 \ldots, A_{[k]}^k$ are linearly independent (since $\rho^{(k)} \neq 0$ is the $k$th leading principal minor of non-singular $A$).
The REF LU factorization of $A$, henceforth abbreviated as REF-LU($A$), is an LD$^{-1}$U factorization, that is, it consists of a lower-triangular matrix $L$, the inverse of a diagonal matrix $D$, and an upper-triangular matrix $U$. The contents of the three matrix factors are obtained from the iterative entries of the IPGE algorithm applied to $A$ and are given by:

\begin{align*}
l_{i,j} &= a_{i,j}^{(j-1)}, \quad \text{for } i \geq j; \\
d_{i,i} &= \rho^{(i-1)} \rho^{(i)} a_{i-1,i-1}^{(i-2)} a_{i,i}^{(i-1)}, \quad \text{for all } i; \quad \text{and} \\
u_{i,j} &= a_{i,j}^{(i-1)}, \quad \text{for } i \leq j;
\end{align*}

where $1 \leq i, j \leq n$. However, $D$ does not need to be stored. Its entries can be generated from the diagonal of $L$ or $U$—specifically, $a_{i-1,i-1}^{(i-2)} = l_{i-1,i-1} = u_{i-1,i-1}$ and $a_{i,i}^{(i-1)} = l_{i,i} = u_{i,i}$, where it is assumed that $a_{0,0}^{(-1)} := \rho^{(0)} = 1$. When $A$ is symmetric, $U = L^T$, thereby inducing the REF Cholesky factorization, whose exact expression is given by $(LD^{-1/2})(LD^{-1/2})^T$.

REF forward substitution on a vector $b$ is performed with the lower-triangular factor $L$ of REF-LU($A$) by initializing and then iteratively updating vector $y \in \mathbb{Z}^n$, for iterations $k = 0, \ldots, n-1$, as follows:

\begin{align*}
y_i &= \begin{cases} 
   b_i & \text{if } k = 0, \\
   l_{1,1} y_i - l_{i,1} y_1 & \text{if } k = 1, \\
   \frac{(l_{i,k} y_{i-k+1} - l_{i,i} y_k)}{l_{k,k-1}} & \text{otherwise}
\end{cases} \\
   \text{for } i = k+1 \ldots n.
\end{align*}

The output vector is the solution to the SLE $LD^{-1}y = b$ or, equivalently, $y = (LD^{-1})^{-1}b$. However, to solve $Ax = b$ in full without roundoff errors, REF forward and backward substitution must be applied on the scaled SLE $Ax' = b'$, where $x' = \det(A)x$ and $b' = \det(A)b$. The forward substitution vector $y'$ for the scaled system $LD^{-1}y' = b'$ is equivalently obtained without roundoff errors by evaluating (7) and setting $y' = \det(A)y = l_{n,n}y$.

Having obtained $y'$, REF backward substitution is performed as follows:

\begin{align*}
x'_i &= \frac{1}{u_{i,i}} \left( y'_i - \sum_{j=i+1}^{n} u_{i,j} x'_j \right) \quad \text{for } i = n \ldots 1.
\end{align*}

Afterward, the exact solution to the original SLE can reported to any desired precision through the equation:

\begin{align*}
x_i &= \frac{x'_i}{\det(A)} = \frac{x'_i}{l_{n,n}} \quad \text{for } i = 1 \ldots n.
\end{align*}
Before proceeding, it is important to state that the worst-case computational complexities (WCC) of IPGE, REF factorization, and REF substitution are as follows:

\[
\text{WCC(IPGE/REF factorization)} = O(n^3(\beta_{\text{max}} \log \beta_{\text{max}} \log \log \beta_{\text{max}})) \tag{10}
\]

\[
\text{WCC(REF substitution)} = O(n^2(\beta_{\text{max}} \log \beta_{\text{max}} \log \log \beta_{\text{max}})). \tag{11}
\]

In Equations (10) and (11), the WCC measures use the bit-length bound \( \beta_{\text{max}} \) from the IPGE algorithm to account for the added complexity of operand growth in the exact factorization’s entries. The expression in the innermost parentheses of both equations represents the cost of multiplying/dividing two integers of bit-length \( \beta_{\text{max}} \) according to FFT techniques \( \text{[Schönhage and Strassen 1971 Knuth 1981]} \); the quantity outside the innermost parentheses represents the algorithms’ number of operations.

### 2.3. Updating the REF Factorizations

Escobedo and Moreno-Centeno (2017) introduced algorithms for performing various LP-related updates on the REF LU and Cholesky factorizations, namely, addition, deletion, and replacement of a single row/column of \( A \). The push-and-swap column replacement approach developed therein contrasts with the traditional delete-insert-reduce update approach, although they both require \( O(n^2) \) operations. The latter approach immediately deletes the exiting column, inserts the incoming column in a strategic position, and performs row-reduction operations to return the factors to triangular form (for a survey of various update algorithms that can be categorized under the delete-insert-reduce approach, we refer the reader to Elble and Sahinidis (2012)). Applying this traditional approach on the REF factorizations leads to a loss in the information that was used to guarantee exact divisibility during each iteration of the factorization process. Without this information, the IPGE pivoting process must be restarted to guarantee exact divisibility in the new row reduction operations, causing prohibitive increases in computational effort—in fact, the update times can exceed the factorization run-times by close to two orders of magnitude for small-to-moderate size matrices. Conversely, the push-and-swap column replacement approach preserves the special structure of the REF factorization by repeatedly permuting the column exiting the basis with its right-adjacent column until it is pushed out of the factorization and replaced with the (updated) incoming column. This special procedure avoids growth in the encoding size of the matrix entries, specifically, it ensures the entries of the updated factorization retain the bit-length bound \( \beta_{\text{max}} \) (see Section 2.2).
A crucial distinction of a rank-one update is that most, if not all, columns of \( A \) change at once rather than a single row or column, when the operation defined in (1) is applied to yield \( \hat{A} \). This means that, while \( \text{REF-LU}(\hat{A}) \) could be obtained as a sequence of column replacements, doing so would require \( O(n^3) \) operations—\( O(n^2) \) operations for each of \( O(n) \) column updates. This would cancel out the operations savings expected of the factorization update and, therefore, a fundamentally different approach is needed to perform fast and efficient rank-one updates on the REF factorizations. Inefficient algorithms would also result from a direct adaptation of other update algorithms (e.g., Gill et al. (1987), Stange et al. (2007)), that is, through the replacement of their floating-point operations with exact arithmetic. In greater detail, because the division operations that would be involved are not guaranteed to be exact, such implementations would entail switching to exact rational arithmetic. This would effectively eliminate the advantages of integer-preserving arithmetic vis-à-vis the latter methodology of exact computation, which include faster run times and lower memory requirements. We direct the reader to Escobedo et al. (2018), Lourenco et al. (2019) for comparisons of these two exact methodologies for LU factorization and forward/backward substitution on dense and sparse matrices.

3. Theoretical Insights

This subsection derives theoretical insights that have special import with the REF LU and Cholesky factorization algorithms. The ensuing discussion focuses on the simpler update \( \hat{A} = A + vw^T \) without loss of generality, since the scaled outer product \( \gamma v'w^T \) can be expressed as \( vw^T \), where \( v = \gamma v' \) and \( v' \in \mathbb{Z}^n \). The next two theorems introduce new identities of the adjoint matrix, \( \text{adj}(\cdot) \). Then, an ensuing corollary connects these identities to the IPGE algorithm, from which the entries of the REF-LU factorization are obtained (see Section 2.2). Note that although this work assumes that \( A \in \mathbb{Z}^{n \times n}, \ v, w \in \mathbb{Z}^n \), and \( \gamma \in \mathbb{Z}^1 \), the theoretical results presented in this section extend to rational- and real-numbered matrices.

**Theorem 1.** Let \( A \) be nonsingular. Then, the following identity holds:

\[
\text{adj}(A)v = \text{adj}(A + vw^T)v.
\]

**Proof.** The adjoint matrices of \( A \) and \( A + vw^T \) are related through the equation (Elsner and Rozsa 1981):

\[
\text{adj}(A + vw^T) = \text{adj}(A) + w^T \text{adj}(A)vA^{-1} - \text{adj}(A)vw^TA^{-1} \quad (12)
\]

\[
\Rightarrow \text{adj}(A + vw^T) - \text{adj}(A) = [w^T \text{adj}(A)vI_n - \text{adj}(A)vw^T]A^{-1}, \quad (13)
\]
where $I_n$ is the identity matrix of order $n$. Multiplying by $v$ from the right gives:

$$\text{adj}(A + vv^T)v - \text{adj}(A)v = [w^T\text{adj}(A)v I_n - \text{adj}(A)vw^T] A^{-1}v.$$  

Therefore, the desired result is established by demonstrating that

$$[w^T\text{adj}(A)v I_n - \text{adj}(A)vw^T] A^{-1}v = 0_n \quad \text{(14)}$$

$$\Leftrightarrow [w^T\text{adj}(A)v I_n - \text{adj}(A)vw^T] \text{adj}(A)v = 0_n \quad \text{(15)}$$

where $0_n$ is the zero-vector of size $n$. This is shown by redistributing the left-hand side of (15) as:

$$[w^T\text{adj}(A)v] \text{adj}(A)v - [\text{adj}(A)vw^T] \text{adj}(A)v = [w^T\text{adj}(A)v] \text{adj}(A)v - \text{adj}(A)v [w^T\text{adj}(A)v] = 0_n, \quad \text{(16)}$$

where the first equality in (16) uses the associativity of matrix multiplication.

**Theorem 2.** Let $A$ be nonsingular. Then, the following identity holds:

$$w^T \text{adj}(A) = w^T \text{adj}(A + vv^T).$$

**PROOF.** Similar to Theorem 1, we begin with the difference between the adjoint matrix of $A$ and of its rank-one update (see (13)), which multiplied from the left by $w^T$ gives:

$$w^T \text{adj}(A + vv^T) - w^T \text{adj}(A) = w^T [w^T\text{adj}(A)v I_n - \text{adj}(A)vw^T] A^{-1}$$

In this case, the desired result is established by demonstrating that

$$w^T [w^T\text{adj}(A)v I_n - \text{adj}(A)vw^T] A^{-1} = 0_n \quad \text{(17)}$$

$$\Leftrightarrow w^T [w^T\text{adj}(A)v I_n - \text{adj}(A)vw^T] \text{adj}(A) = 0_n. \quad \text{(18)}$$

This is shown by reorganizing the left-hand side of the latter equation, culminating with the expression:

$$w^T [w^T\text{adj}(A)v] \text{adj}(A) - [w^T\text{adj}(A)v] w^T \text{adj}(A) = 0. \quad \text{(19)}$$

**Corollary 1.** Let $x'$ denote the vector obtained from performing REF forward substitution (see (7)), followed by REF backward substitution (see (8)) with REF-LU($A$) on $v' := \text{det}(A)v$. Additionally, let $x''$ denote the vector obtained by performing REF forward substitution, followed by REF backward substitution, with REF-LU($\hat{A}$) on $v'' := \text{det}(\hat{A})v$. It must be the case that $x' = x''$.

**PROOF.** From the given information, $x'$ and $x''$ satisfy the respective SLEs $Ax' = v'$ and $\hat{A}x'' = v''$. Based on the properties of REF backward substitution, we have that:

$$x' = \text{det}(A)x = \text{det}(A)A^{-1}v = \text{adj}(A)v = \text{adj}(\hat{A})v = \text{det}(\hat{A})\hat{x} = x''.$$

The ensuing theorems extend the implications of this result, which in and of itself is insufficient for reconstructing REF-LU($\hat{A}$) from REF-LU($A$). To continue, it is convenient to state a basic identity.

**Proposition 1.** For any nonsingular lower-triangular matrix $\Lambda \in \mathbb{R}^{n \times n}$,

$$(\Lambda^{-1})^{[k]}_{[k]} = (\Lambda^{[k]}_{[k]})^{-1}. \quad \text{(20)}$$

That is, the first $k$ rows and columns of $\Lambda^{-1}$ are exactly the inverse of the submatrix induced by the first $k$ rows and columns of $\Lambda$. 

Theorem 3. Let $LD^{-1}U$ and $\hat{L}\hat{D}^{-1}\hat{U}$ be the REF-LU factorizations of $A$ and $\hat{A} = A + vw^T$, respectively. The result of applying forward substitution on $v$ using $L$ matches the result of applying forward substitution on $v$ using $\hat{L}$, that is,

$$(LD^{-1})^{-1}v = (\hat{L}\hat{D}^{-1})^{-1}v.$$ 

Proof. The adjoint matrix $\text{adj}(A)$ can be re-expressed using REF-LU($A$) as:

$$\text{adj}(A) = \text{det}(A)A^{-1} = \text{det}(A)(LD^{-1}U)^{-1} = \text{det}(A)U^{-1}(LD^{-1})^{-1}.$$ 

From these equations, the $n$th row of $\text{adj}(A)$, written succinctly as $(\text{adj}(A))_n^{[n]}$, is given by

$$(\text{adj}(A))_n^{[n]} = \text{det}(A)(U^{-1})_n^{[n]}(LD^{-1})^{-1} = \text{det}(A)[0 0 \ldots 0 1/u_{m,m}](LD^{-1})^{-1} = u_{m,m}[0 0 \ldots 0 1/u_{m,m}](LD^{-1})^{-1} = e_n^T(LD^{-1})^{-1} = (LD^{-1})^{-1}_n^{[n]};$$

where $e_n^T$ is the $n$th elementary vector of length $n$. To extend this analysis to characterize an arbitrary row of $(LD^{-1})^{-1}$, let $L(A_{[k]}^k)$ and $D^{-1}(A_{[k]}^k)$ be the lower-triangular matrix and diagonal matrix corresponding to REF-LU($A_{[k]}^k$), that is, the REF LU factorization of the (nonsingular) submatrix induced by the first $k$ rows and columns of $A$. Since the product $LD^{-1}$ is nonsingular and lower-triangular, the inverse matrices $\left(L(A_{[k]}^k)D^{-1}(A_{[k]}^k)\right)^{-1}$ nest atop one another as $k$ increases per Proposition 1 meaning that the following relationship holds, for $k = 1, \ldots, n$:

$$(LD^{-1})^{-1}_{[k]} = \left(L(A_{[k]}^k)D^{-1}(A_{[k]}^k)\right)^{-1}. \quad (21)$$

From the preceding series of equations, this implies that the $k$th row of matrix $(LD^{-1})^{-1}$ can be written as

$$\left((LD^{-1})^{-1}\right)_k^{[k]} = \left[\text{adj}(A)_{[k]}^{[k]}\right]_k^{[k]}0_{n-k}^T,$$

where $0_{n-k}^T$ is the (row) 0-vector of dimension $n-k$. Lastly, applying Theorem 3 gives that:

$$\left(\text{adj}(A)_{[k]}^{[k]}\right)_k^{[k]}v = \left(\text{adj}(A)_{[k]}^{[k]}\right)_k^{[k]}v,$$

for $k = 1, \ldots, n$, thereby establishing the desired result. □

Theorem 4. Let $LD^{-1}U$ and $\hat{L}\hat{D}^{-1}\hat{U}$ be the REF-LU factorizations of $A$ and $\hat{A} = A + vw^T$, respectively. The result of applying forward substitution on $w$ using $U$ matches the result of applying forward substitution on $w$ using $\hat{U}^T$, that is,

$$(U^TD^{-1})^{-1}w = (\hat{U}^T\hat{D}^{-1})^{-1}w.$$
The REF LU factorizations of $A^T$ and $\hat{A}^T$ are exactly the transpose of the factorizations REF-LU($A$) and REF-LU($\hat{A}$), respectively (Escobedo and Moreno-Centeno 2017). This means that $U^T$ and $\hat{U}^T$ are the corresponding lower triangular matrices needed to perform REF forward substitution on $w$ with REF-LU($A^T$) and REF-LU($\hat{A}^T$). Now, from Theorem 2, we have that:

$$w^T \text{adj}(A) = w^T \text{adj}(\hat{A}).$$
$$\iff \text{adj}(A)^T w = \text{adj}(\hat{A})^T w.$$
$$\iff \text{adj}(A^T) w = \text{adj}(\hat{A}^T) w.$$

Therefore, the desired result is obtained through a parallel line of arguments as Theorem 3. □

Theorems 3 and 4 prove that performing REF forward substitution on $v$ (on $w$, resp.) with REF-LU($A$) or with REF-LU($\hat{A}$) (with REF-LU($A^T$) or with REF-LU($\hat{A}^T$), resp.) yields identical results. It is necessary to go one step further and show that the intermediary update vectors calculated during this algorithm, with either the original or updated factorizations, also match. To that end, we introduce a stepwise recursion of REF forward substitution in Algorithm 1, denoted succinctly as REF-FS-Step. In words, Algorithm 1 receives the forward substitution vector from step $k-1$ (say $y^{(k-1)}$), column $k$ of $L$ (say $L^k_{[n]}$), the pivot used in step $k-1$ ($\rho^{(k-1)} = l_{k-1,k-1}$), and the iteration counter ($k$); it uses these inputs to calculate and return the forward substitution vector for step $k$, where $1 \leq k \leq n-1$. Therefore, running the original REF forward substitution algorithm on the update vector $v$ with REF-LU($A$) is equivalent to performing the recursion $y^{(k)} = \text{REF-FS-Step}(y^{(k-1)}, L^k_{[n]}, l_{k-1,k-1}, k)$, for $k = 1, \ldots, n-1$, where $y^{(0)} = v$.

Algorithm 1: REF Forward Substitution Recursive Step (REF-FS-Step)

```
input : $y^{(k-1)}$, $L^k_{[n]}$, $\rho^{(k-1)}$, $k$
let $y^{(k)} \in \mathbb{Z}^n$
for $i = k + 1, \ldots, \left|y^{(k-1)}\right|$ do
    $y_i^{(k)} = l_{k,k} y_i^{(k-1)} - l_{i,k} y_k^{(k-1)}$
if $k > 0$ then
    $y_i^{(k)} \leftarrow y_i^{(k)} / \rho^{(k-1)}$
return $y^{(k)}$
```

Theorem 5. The intermediary forward substitution vectors $y^{(k)}$ and $\hat{y}^{(k)}$ obtained at the conclusion of the $k$th iteration of REF forward substitution on $v$ using $L$ and $\hat{L}$, respectively, are equal, for $k = 1, \ldots, n-1$.

Proof. Upon completion of the $k$th iteration of REF forward substitution, the individual elements of $y^{(k)}$ are connected to IPGE entries according to the equation (Escobedo and Moreno-Centeno 2015):

$$y_i^{(k)} = \begin{cases} a_{i,n+1}^{(k)} & \text{if } i \leq k \\ a_{i,n+1}^{(k)} & \text{if } i > k \end{cases}$$

(22)
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where column \(n+1\) of \(A\) denotes the right-hand vector on which IPGE is applied (\(v\) in this theorem). Based on this connection, each element \(i > k \geq 1\) of \(y^{(k)}\) can be equivalently obtained as

\[
y^{(k)}_i = \left( L(A^{[k+1]}_{[k],i})D(A^{[k+1]}_{[k],i})^{-1} \right)^{-1} v_{[k],i},
\]

where \(L(A^{[k+1]}_{[k],i})\) and \(D(A^{[k+1]}_{[k],i})^{-1}\) are the lower-triangular and diagonal matrices corresponding to the REF-LU factorization of the (nonsingular) submatrix induced by columns \([k+1] = \{1, \ldots, k+1\}\) and rows \([k] \cup i = \{1, \ldots, k, i\}\) of \(A\). The above equation can be understood from the observations that element \(k+1\) of \(y\) does not change after iteration \(k\) of the algorithm and that, if any row \(i > k\) of \(A\) and \(y\) is swapped with row \(k+1\), the new element \(k+1\) of \(y\) at iteration \(k\) can be obtained using the inverse of the REF lower-triangular and diagonal matrices of the corresponding submatrix of \(A\). Furthermore, from the basic identity given by Proposition \[1\]

\[
\left( L(A^{[k+1]}_{[k],i})D(A^{[k+1]}_{[k],i})^{-1} \right)^{-1} = \left( (LD^{-1})^{-1} \right)^{[k+1]}_{[k],i},
\]

where \(1 \leq k < i\). Piecing this together with the above analysis, each entry of \(y^{(k)}\) is given by

\[
y^{(k)}_i = \begin{cases} 
\left( \text{adj}(A)_{[i]} \right)_i v_{[i]} & \text{if } i \leq k \\
\left( \text{adj}(A)_{[k+1]} \right)_{k+1} v_{[k],i} & \text{if } i > k.
\end{cases}
\]

Since each \(y^{(k)}_i\) (\(\hat{y}^{(k)}_i\), resp.) is the product of the bottom row of the adjoint matrix of a submatrix of \(A\) (\(\hat{A}\), resp.) and a subvector of \(v\), the proof is completed based on a similar reasoning as Theorem \[5\].

**Theorem 6.** The intermediary forward substitution vectors \(z^{(k)}\) and \(\hat{z}^{(k)}\) obtained at the conclusion of the \(kth\) iteration of REF forward substitution on \(w\) using \(U^T\) and \(\hat{U}^T\), respectively, are equal, for \(k = 1, \ldots, n-1\).

**Proof.** The result is obtained through the combined logic of Theorems \[4\] and \[5\].

4. **REF Rank-One Update Algorithm**

This sections introduces and proves the correctness of the featured algorithms and is organized as follows. Section \[4.1\] derives a standard version of the REF rank-one update algorithm, which relies on certain assumptions, and Section \[4.2\] walks through a numerical example. Then, Section \[4.3\] derives adjustments for dealing with cases when the standard algorithm fails (i.e., when its assumptions do not hold).

4.1. **Standard Version**

The pseudocode of the REF rank-one update algorithm, denoted succinctly as REF-ROU, is given in Algorithm \[2\]. Its steps and their validity are further described in the accompanying proof of correctness and computational complexity. The ensuing lemma is needed for said proof.

**Lemma 1.** Let \(L\) be the lower-triangular matrix factor of the REF-LU factorization of nonsingular matrix \(A\), and let \(y^{(k)}\) denote the vector output after the \(kth\) iteration of the stepwise recursion of REF forward substitution performed on a vector \(v\) using \(L\). The following division is exact:

\[
\frac{l_{k,k} y^{(k-1)}_i - l_{k-1,k} y^{(k-1)}_i}{y^{(k-1)}_i},
\]

where \(2 \leq k < i \leq n\).
PROOF. Entry $l_{i,k} \in \mathbb{Z}^1$ can be expanded as

$$l_{i,k} = \frac{l_{i,k}y_k^{(k-1)}}{y_k^{(k-1)}}$$  \hspace{1cm} (25)

$$= \frac{l_{i,k}y_k^{(k-1)} + l_{k,k}y_i^{(k-1)} - l_{i,k}y_i^{(k-1)}}{y_k^{(k-1)}}$$  \hspace{1cm} (26)

$$= \frac{l_{k,k}y_i^{(k-1)} - \left(l_{k,k}y_i^{(k-1)} - l_{i,k}y_i^{(k-1)}\right)}{y_k^{(k-1)}}$$  \hspace{1cm} (27)

$$= \frac{l_{k,k}y_i^{(k-1)} - l_{k-1,k-1}y_i^{(k)}}{y_k^{(k-1)}}.$$  \hspace{1cm} (28)

The division in the right-hand side of Equation (25) is clearly exact. Its result matches Equations (26) and (27), since in the former the terms added to the numerator cancel out, and in the latter the three numerator terms are only reorganized. Equation (28) results from the stepwise recursion of REF forward substitution (see Algorithm 1); namely, from the formula $\hat{A} = \hat{L} \hat{D} \hat{U}$, the expression within the parenthesis of Equation (27) is substituted with $l_{k-1,k-1}y_i^{(k)}$, which is a product of two integer entries. Based on the above series of equations, the Equation (28) numerator is a multiple of the denominator. \qed

**Theorem 7.** Define matrices $A$ and $\hat{A}$ and update vectors $v$ and $w$ as in Assumption 7 and let $REF-LU(A) = LD^{-1}U$ and $REF-LU(\hat{A}) = \hat{L} \hat{D}^{-1} \hat{U}$. Additionally, let $y^{(k)}$ and $z^{(k)}$ denote the vectors output after the $k$th iteration of the stepwise recursion of REF forward substitution performed on $v$ using $L$ and on $w$ using $U^T$, respectively, for $k = 1, \ldots, n-1$. Under the assumption that $y_k^{(k-1)} \neq 0$ and $z_k^{(k-1)} \neq 0$, for $k = 2, \ldots, n-1$, Algorithm 2 successfully obtains $REF-LU(\hat{A})$ from $REF-LU(A)$ without roundoff errors in $O(n^2)$ operations.

**PROOF.** First, we explain how to obtain the off-diagonal entries of $REF-LU(\hat{A})$, whose calculation requires the availability of the updated factorization pivots (i.e., $\hat{p}^k := \hat{l}_{k,k} = \hat{u}_{k,k}$); afterward, we explain how the diagonal of $REF-LU(\hat{A})$ is iteratively constructed along the update process to furnish the required pivots.

Since the entries along the first row and column of a $REF-LU$ factorization match the respective input matrix entries, the first row and column of $REF-LU(\hat{A})$ are obtained by simply adding $v_1 w_1$ to $u_{1,i} = a_{1,i}^{(0)}$ and $v_i w_1$ to $l_{i,1} = a_{i,1}^{(0)}$, for $i = 2, \ldots, n$; this is accomplished with the initial for-loop (its first and second statements) without roundoff errors in $O(n)$ operations. The bulk of the off-diagonal entries are obtained by utilizing the theoretical insights derived in Section 3. In particular, Theorem 5 establishes that $y^{(k)}$ can be equivalently obtained from the $k$th step of $REF$ forward substitution on $v$ using either $L$ or $\hat{L}$ as the lower-triangular matrix factor; similarly, Theorem 6 establishes that $z^{(k)}$ can be equivalently obtained from the $k$th step of $REF$ forward substitution on $w$ using either $U^T$ or $\hat{U}^T$. The ensuing arguments leverage the first of these two insights to reconstruct the entries of $\hat{L}$ from the outputs of $REF$ forward substitution using $L$; parallel arguments are used to reconstruct the entries of $\hat{U}^T$ from the outputs of $REF$ forward substitution using $U^T$, but they are omitted for brevity. From the stepwise recursion of $REF$ forward substitution, each entry $y_i^{(k)}$ is obtainable using $\hat{L}$ as

$$y_i^{(k)} = \frac{\hat{l}_{i,k}y_i^{(k-1)} - \hat{l}_{i,k}y_i^{(k-1)}}{l_{k-1,k-1}},$$
Algorithm 2: REF Rank-one Update Algorithm (REF-ROU)

input : $L, U, v, w, \text{Diag}(A)$

let $\hat{L}, \hat{U} \in \mathbb{Z}^{n \times n}$

$\hat{l}_{1,1}, \hat{u}_{1,1} = a_{1,1} + v_1 w_1$

for $i = 2, \ldots, n$ do

$\hat{u}_{i,i} = u_{1,i} + v_1 w_i$

$\hat{l}_{i,1} = l_{i,1} + v_i w_1$

$\hat{l}_{i,i}, \hat{u}_{i,i} = a_{i,i} + v_i w_i$

$y^{(1)} = \text{REF-FS-Step}(y^{(0)} = v, L^1_{[n]}, 1, 1)$

$z^{(1)} = \text{REF-FS-Step}(z^{(0)} = w, (U^T)^1_{[n]}, 1, 1)$

for $k = 2, \ldots, n-1$ do

$y^{(k)} = \text{REF-FS-Step}(y^{(k-1)}, L^k_{[n]}, l_{k-1,k-1}, k)$

$z^{(k)} = \text{REF-FS-Step}(z^{(k-1)}, (U^T)^k_{[n]}, u_{k-1,k-1}, k)$

for $i = k, \ldots, n$ do

$\hat{l}_{i,i}, \hat{u}_{i,i} \leftarrow [\hat{l}_{i-1,k-1}\hat{l}_{i,i} - (\hat{u}_{k-1,i}\hat{l}_{i,k-1})] / \hat{l}_{k-2,k-2}$

if $i > k$ then

$\hat{l}_{i,k} = [(\hat{l}_{k,k}y^{(k-1)}_i - (\hat{l}_{k-1,k-1}y^{(k)}_i))/y^{(k-1)}_k$

$\hat{u}_{k,i} = [(\hat{u}_{k,k}z^{(k-1)}_i - (\hat{u}_{k-1,k-1}z^{(k)}_i))/z^{(k-1)}_k$

$\hat{l}_{n,n}, \hat{u}_{n,n} \leftarrow [(\hat{l}_{n-1,n-1}\hat{l}_{n,n}) - (\hat{u}_{n-1,n}\hat{u}_{n,n-1})] / \hat{l}_{n-2,n-2}$

return $\hat{L}, \hat{U}$

where $i > k$ and $\hat{l}_{0,0} = 1$. Reorganizing this expression to isolate $\hat{l}_{i,k}$ gives

$$\hat{l}_{i,k} = \frac{\hat{l}_{k,k}y^{(k-1)}_i - \hat{l}_{k-1,k-1}y^{(k)}_i}{y^{(k-1)}_k}.$$  

In words, for each $k = 2, \ldots, n-1$, column $k$ of $\hat{L}$ is reconstructed from the iteration $k-1$ and $k$ REF forward substitution vectors—$y^{(k-1)}$ and $y^{(k)}$, obtained using $L$—and from updated pivots—$\hat{l}_{k-1,k-1}$ and $\hat{l}_{k,k}$ (see next paragraph); these four required components are calculated (or already available) at the start of the $k$th iteration of the outer for-loop of the algorithm. Because $y^{(k-1)}_k \neq 0$, from the given assumption, and the above division is exact, according to Lemma 1, $\hat{l}_{i,k}$ is successfully obtained free of roundoff error. Moreover, since each call to the stepwise recursion of REF forward substitution in the outer for-loop and each full execution of the inner for-loop requires $O(n)$ operations, updating the off-diagonal entries along rows and columns $[n]\{1\}$ of REF-LU($A$) requires $O(n^2)$ operations.

REF-ROU obtains the updated factorization pivots as follows. First, Diag($\hat{A}$) is obtained directly from Diag($A$) in the initial for-loop (its third statement). This opening step provides the correct and final value of
the first updated pivot \((\hat{\rho}^1 = \hat{l}_{1,1} = \hat{u}_{1,1})\), and it populates starting values for diagonal elements \(i = 2, \ldots, n\), which will be finalized one by one in subsequent iterations. In the next for-loop (which starts at \(k = 2\)), the initial step of the inner for-loop provides the correct and final value of the second updated diagonal element \((\hat{\rho}^2 = \hat{l}_{2,2} = \hat{u}_{2,2})\); this is established by the fact that the right-hand side of its first statement can be written in terms of IPGE entries as

\[
\hat{l}_{1,1} \hat{l}_{2,2} - \hat{u}_{1,2} \hat{u}_{2,1} = \frac{\hat{a}_{1,2}^{(0)} \hat{a}_{2,2}^{(0)} - \hat{a}_{1,2}^{(0)} \hat{a}_{2,1}^{(0)}}{\hat{a}_{0,0}^{(-1)}} = \hat{a}_{2,2}^{(1)} = \hat{\rho}^2.
\]

Similarly, upon completion of the first outer for-loop iteration, the \(i\)th diagonal entry is equivalent to entry \(\hat{a}_{1,i}^{(1)}\), where \(3 \leq i \leq n\), meaning these entries have been advanced from iteration 0 to iteration 1 of IPGE and are not yet in their final form. Continuing with this process, upon completion of outer for-loop iteration \(k\), diagonal entry \(\hat{l}_{i,i}\) with \(i > k\) is equivalent to \(\hat{a}_{i,i}^{(k-1)}\); hence, \(\hat{\rho}^k = \hat{l}_{k,k} = \hat{u}_{k,k}\) is finalized during this iteration. The entries required to obtain this IPGE entry are available to the algorithm since

\[
\hat{a}_{i,i}^{(k-1)} = \frac{\hat{a}_{k-1,i}^{(k-2)} - \hat{a}_{k-1,i}^{(k-2)} \hat{a}_{i,k-1}^{(k-2)}}{\hat{a}_{k-2,k-2}^{(k-3)}} = \frac{\hat{l}_{k-1,k-1}^{(k-2)} \hat{a}_{i,k-1}^{(k-2)} - \hat{u}_{k-1,k-1}^{(k-2)} \hat{l}_{i,k-1}^{(k-2)}}{\hat{l}_{k-2,k-2}^{(k-3)}},
\]

where the second equation is obtained from the relationship between \(\text{REF-LU}(\hat{A})\) and the iterative entries of the IPGE algorithm. That is, the entries involved in the calculation of \(\hat{a}_{i,i}^{(k-1)}\) are drawn from the updated pivots of the previous two iterations and from column \(k-1\) of \(\hat{L}\) and row \(k-1\) of \(\hat{U}\), both obtained during iteration \(k-1\) of the outer for-loop (along with \(\hat{a}_{i,i}^{(k-2)}\)). Since the final updated pivot \((\rho^{(n)} = \hat{l}_{n,n} = \hat{u}_{n,n})\) is calculated using a similar string of operations culminating in the last line of the algorithm, the updated pivots \(\hat{\rho}^k = \hat{a}_{k,k}^{(k-1)}\) are calculated correctly using roundoff-error free operations, for \(k = 1, \ldots, n\). For each iteration of the outer for-loop, \(O(n)\) operations are required to perform an IPGE step on the full diagonal. Therefore, \(O(n^2)\) operations are required to obtain all updated pivots and to perform the full rank-one update. \(\square\)

The ensuing corollary provides the worst-case computational complexity of the REF rank-one update algorithm (abbreviated as WCC(REF-ROU)). The analysis combines the algorithm’s \(O(n^2)\) required operations and the cost of multiplying/dividing two integers with bit-length \(\hat{\beta}_{\text{max}} \leq \lceil \log(\sigma \sqrt{n}) \rceil\), where \(\sigma := \max_{i,j} \{ \max(|a_{i,j}^{(0)}|, |a_{i,j}^{(0)}|) \}\). The latter costs must be incorporated since the REF algorithms entail working with matrix entries with non-fixed precision.

**Corollary 2.** The worst-case computational complexity (WCC) of REF-ROU is given by:

\[
\text{WCC(REF-ROU)} = O(n^2(\hat{\beta}_{\text{max}} \log \hat{\beta}_{\text{max}} \log \log \hat{\beta}_{\text{max}})) = O(n^2 \max(\log^2 n \log \log n, \log^2 \sigma \log \log \sigma)).
\]

It is worth adding that the bound on \(\hat{\beta}_{\text{max}}\) is somewhat pessimistic (Abbott and Mulders 2001; Cook and Steffy 2011), meaning that the algorithms perform more efficiently in practice than this theoretical measure suggests. Furthermore, it is reasonable to expect efficiency gains when the algorithms are adapted for sparse and other well structured matrices occurring in real-world applications (see Lourenco et al. 2019).
4.2. Numerical Example

This subsection provides a numerical application of the REF-ROU algorithm. To start, consider the following input matrix \( A \in \mathbb{Z}^{4\times 4} \), its REF LU factorization, and update vectors \( v, w \in \mathbb{Z}^4 \):

\[
A = \begin{bmatrix}
3 & 8 & 7 & 1 \\
5 & 3 & 5 & 4 \\
6 & -2 & 1 & 7 \\
7 & -2 & -6 & 11
\end{bmatrix}, \quad \text{REF-LU}(A) = \begin{bmatrix}
3 & 8 & 7 & 1 \\
5 & -31 & -20 & 7 \\
6 & -54 & 43 & -29 \\
7 & -62 & 279 & -89
\end{bmatrix}, \quad v = \begin{bmatrix}
1 \\
5 \\
7 \\
2
\end{bmatrix}, \quad w = \begin{bmatrix}
2 \\
6 \\
3 \\
4
\end{bmatrix}.
\]

REF-LU(\( A \)) above is displayed in a succinct form that merges together the \( L \) and \( U \) matrices; this is possible because the diagonals of both matrices are identical and the algorithm does not have need for the \( D \) matrix.

From these inputs, the rank-one matrix \( vw^T \), the update matrix \( \hat{A} \), and the REF LU factorization of \( \hat{A} \) (i.e., the desired output from REF-ROU) are as follows:

\[
vw^T = \begin{bmatrix}
2 & 6 & 3 & 4 \\
10 & 30 & 15 & 20 \\
14 & 42 & 21 & 28 \\
4 & 12 & 6 & 8
\end{bmatrix}, \quad \hat{A} = \begin{bmatrix}
5 & 14 & 10 & 5 \\
15 & 33 & 20 & 24 \\
20 & 40 & 22 & 35 \\
11 & 10 & 0 & 19
\end{bmatrix}, \quad \text{REF-LU}(\hat{A}) = \begin{bmatrix}
5 & 14 & 10 & 5 \\
15 & -45 & -50 & 45 \\
20 & -80 & 10 & 45 \\
11 & -104 & -50 & -178
\end{bmatrix}.
\]

Next, we describe how to obtain \( \text{REF-LU}(\hat{A}) \) by updating \( \text{REF-LU}(A) \). The walk-through is divided into four parts: initial steps, outer for-loop iteration \( k = 2 \), outer for-loop iteration \( k = 3 \), and final step. For convenience, the entries of \( \text{REF-LU}(\hat{A}) \) that are finalized after each part are bolded and colored in blue.

**Initial Steps.** Begin by constructing the entries along the first row and column of \( \text{REF-LU}(\hat{A}) \), by taking the matching entries of \( A \) and adding the corresponding product of entries from \( v \) and \( w \). The specific calculations are as follows:

\[
\hat{u}_{12} = a_{12} + v_1w_2 = 8 + 1(6) = 14 = 7 + 1(3) = 10 = 1 + 1(4) = 5 \\
\hat{u}_{13} = a_{13} + v_1w_3 = 7 + 1(3) = 10 \\
\hat{u}_{14} = a_{14} + v_1w_4 = 1 + 1(4) = 5 \\
\hat{l}_{21} = a_{21} + v_2w_1 = 5 + 5(2) = 15 \\
\hat{l}_{31} = a_{31} + v_3w_1 = 6 + 7(2) = 20 = 7 + 2(2) = 11.
\]

Perform similar operations to obtain the initial elements of the working diagonal of \( \hat{A} \):

\[
\hat{l}_{11} = a_{11} + v_1w_1 = 3 + 1(2) = 5 \\
\hat{l}_{22} = a_{22} + v_2w_2 = 3 + 5(6) = 33 = 1 + 7(3) = 22 \\
\hat{l}_{33} = a_{33} + v_3w_3 = 11 + 2(4) = 19.
\]

Next, calculate the forward substitution vectors for iteration \( k = 1 \), \( y^{(1)} \) and \( z^{(1)} \) using Algorithm 1 and vectors \( y^{(0)} = v \) and \( z^{(0)} = w \), respectively. At the end of these steps, these two vectors and the working factorization, denoted as \( \hat{L}\hat{U} \), are given by:
\[
\begin{align*}
\mathbf{y}^{(1)} &= \begin{bmatrix} 1 \\ 10 \\ 15 \\ -1 \end{bmatrix}, \\
\mathbf{z}^{(1)} &= \begin{bmatrix} 2 \\ 2 \\ -5 \\ 10 \end{bmatrix}, \\
\hat{L} \hat{U} &= \begin{bmatrix} 5 & 14 & 10 & 5 \\ 15 & 33 & \cdot & \cdot \\ 20 & \cdot & 22 & \cdot \\ 11 & \cdot & 19 & \cdot \end{bmatrix}.
\end{align*}
\]

Outer for-loop iteration \( k = 2 \). First, calculate the forward substitution vectors for iteration \( k = 2 \), \( \mathbf{y}^{(2)} \) and \( \mathbf{z}^{(2)} \), using Algorithm \ref{alg} and vectors \( \mathbf{y}^{(1)} \) and \( \mathbf{z}^{(1)} \), respectively. The resulting vectors are given by:

\[
\begin{align*}
\mathbf{y}^{(2)} &= \begin{bmatrix} 1 \\ 10 \\ 25 \\ 217 \end{bmatrix}, \\
\mathbf{z}^{(2)} &= \begin{bmatrix} 2 \\ 2 \\ 65 \\ -108 \end{bmatrix}.
\end{align*}
\]

Second, advance diagonal elements \( \hat{\ell}_{22}, \hat{\ell}_{33}, \hat{\ell}_{44} \) through IPGE pivoting operations:

\[
\begin{align*}
\hat{\ell}_{22} &\leftarrow (\hat{\ell}_{11} \hat{\ell}_{22} - \hat{\ell}_{12} \hat{\ell}_{21})/\hat{\ell}_{00} \\
\hat{\ell}_{33} &\leftarrow (\hat{\ell}_{11} \hat{\ell}_{33} - \hat{\ell}_{13} \hat{\ell}_{31})/\hat{\ell}_{00} \\
\hat{\ell}_{44} &\leftarrow (\hat{\ell}_{11} \hat{\ell}_{44} - \hat{\ell}_{14} \hat{\ell}_{41})/\hat{\ell}_{00}
\end{align*}
\]

\[
\begin{align*}
&= [5(33) - 14(15)]/1 = -45 \\
&= [5(22) - 10(20)]/1 = -90 \\
&= [5(19) - 5(11)]/1 = 40.
\end{align*}
\]

Third, obtain the off-diagonal entries of the second row of \( \hat{U} \) and second column of \( \hat{L} \) through the operations:

\[
\begin{align*}
\hat{u}_{23} &= (\hat{u}_{22} \hat{z}^{(1)}_3 - \hat{u}_{11} \hat{z}^{(2)}_3)/\hat{z}^{(1)}_2 \\
\hat{u}_{24} &= (\hat{u}_{22} \hat{z}^{(1)}_4 - \hat{u}_{11} \hat{z}^{(2)}_4)/\hat{z}^{(1)}_2 \\
\hat{u}_{32} &= (\hat{u}_{22} \hat{y}^{(1)}_3 - \hat{u}_{11} \hat{y}^{(2)}_3)/\hat{y}^{(1)}_2 \\
\hat{u}_{42} &= (\hat{u}_{22} \hat{y}^{(1)}_4 - \hat{u}_{11} \hat{y}^{(2)}_4)/\hat{y}^{(1)}_2
\end{align*}
\]

\[
\begin{align*}
&= [-45(-5) - 5(65)]/2 = -50 \\
&= [-45(10) - 5(-108)]/2 = 45 \\
&= [-45(15) - 5(25)]/10 = -80 \\
&= [-45(-1) - 5(217)]/10 = -104.
\end{align*}
\]

At the end of these steps, the working matrix is given by:

\[
\hat{L} \hat{U} = \begin{bmatrix} 5 & 14 & 10 & 5 \\ 15 & -45 & -50 & 45 \\ 20 & -80 & -90 & \cdot \\ 11 & -104 & \cdot & 40 \end{bmatrix}.
\]

Outer for-loop iteration \( k = 3 \). First, calculate the forward substitution vectors, \( \mathbf{y}^{(3)} \) and \( \mathbf{z}^{(3)} \), using Algorithm \ref{alg} and vectors \( \mathbf{y}^{(2)} \) and \( \mathbf{z}^{(2)} \), respectively. These resulting vectors are given by:

\[
\begin{align*}
\mathbf{y}^{(3)} &= \begin{bmatrix} 1 \\ 10 \\ 25 \\ -76 \end{bmatrix}, \\
\mathbf{z}^{(3)} &= \begin{bmatrix} 2 \\ 2 \\ 65 \\ 89 \end{bmatrix}.
\end{align*}
\]
Second, advance diagonal elements \( \hat{l}_{33} \) and \( \hat{l}_{44} \) through IPGE pivoting operations:

\[
\hat{l}_{33} \leftarrow (\hat{l}_{22}\hat{l}_{33} - \hat{u}_{23}\hat{l}_{32})/\hat{l}_{11} \\
\hat{l}_{44} \leftarrow (\hat{l}_{22}\hat{l}_{44} - \hat{u}_{24}\hat{l}_{42})/\hat{l}_{11}
\]

\[
= [-45(-90) + 50(-80)]/5 = 10 \\
= [-45(40) - 45(-104)]/5 = 576.
\]

Third, obtain the off-diagonal entries of the second row of \( \hat{U} \) and second column of \( \hat{L} \) through the operations:

\[
\hat{u}_{34} = (\hat{u}_{33}\hat{z}_4^{(2)} - \hat{u}_{22}\hat{z}_4^{(3)})/\hat{z}_3^{(2)} \\
= [10(-108) + 45(89)]/65 = 45
\]

\[
\hat{l}_{43} = (\hat{l}_{33}\hat{y}_4^{(2)} - \hat{l}_{22}\hat{y}_4^{(3)})/\hat{y}_3^{(2)} \\
= [10(217) + 45(-76)]/25 = -50.
\]

At the end of these steps, the working matrix is given by:

\[
\hat{L} \backslash \hat{U} = \\
\begin{bmatrix}
5 & 14 & 10 & 5 \\
15 & -45 & -50 & 45 \\
20 & -80 & 10 & 45 \\
11 & -104 & -50 & 576
\end{bmatrix}.
\]

This completes all iterations of the outer for-loop.

**Final step.** Finalize diagonal element \( \hat{l}_{44} \) through an IPGE pivoting operation:

\[
\hat{l}_{44} = (\hat{l}_{33}\hat{l}_{44} - \hat{u}_{34}\hat{l}_{43})/\hat{l}_{22} \\
= [10(576) - 45(-50)]/ -45 = -178.
\]

REF-LU(\( \hat{A} \)) is completed after inserting this updated diagonal element into the previous working matrix.

### 4.3. REF-ROU Special Cases and Adjustments

In its standard form, REF-ROU fails when the division involved in the calculation of the off-diagonal factorization entries is undefined (see equations under the conditional statement of Algorithm 2), due to a zero occurring in a specific element of the iterative update vectors. This subsection introduces adjustments for dealing with two related cases.

**Special Case 1:** Zeros occur before any steps of the algorithm are performed. The problem occurs when the update vectors \( v \) and/or \( w \) contain a leading sequence of zeros. Note that, when zeros occur in these initial vectors after a leading sequence of nonzeros, the rank-one update algorithm tends to turn these entries into nonzeros as it progresses; however, if it does not, Special Case 2 can be applied.

The adjustment consists of two main parts. To describe them, let \( \theta_v \) and \( \theta_w \) be the respective indices of the last zero occurring in an uninterrupted sequence extending from the initial elements of \( v \) and \( w \), that is,

\[
\theta_v = \max_{0 \leq i \leq n} \{ i : v_j = 0 \ \forall j \leq i \} \\
\theta_w = \max_{0 \leq i \leq n} \{ i : w_j = 0 \ \forall j \leq i \}.
\]
where \( v_0 = w_0 = 0 \) by convention, so that \( \theta_v = 0 \) if \( v_1 \neq 0 \) (\( \theta_w = 0 \) if \( w_1 \neq 0 \), resp.). In the first part, all entries of \( \text{REF-LU}(A) \) along rows \([\theta_v] \) and columns \([\theta_w] \) are copied to \( \text{REF-LU}(\hat{A}) \). In the second part, each step of Algorithm 2 is performed in the usual way, with the exception that the inner-for-loop operations are skipped for those entries copied from \( \text{REF-LU}(A) \).

**Special Case 2:** Zeros occur during the execution of the algorithm. The problem occurs when the algorithm encounters \( y_k^{(k-1)} = 0 \) or \( z_k^{(k-1)} = 0 \) at iteration \( k \geq 2 \) of the outer-for-loop. When this happens, it is not possible to evaluate the stated formula for entries \( \hat{l}_{i,k} \) or \( \hat{u}_{k,i} \), respectively, for any \( i > k \). Zeros occurring in other elements of the update vectors at iteration \( k \) do not pose issues.

The adjustment needed to overcome this special case also consists of two main parts; for simplicity, the discussion focuses on \( y_k^{(k-1)} \), since the other case is handled similarly (i.e., in the transpose sense). First, it is necessary to permute either columns \( k-1 \) and \( k \) of \( \text{REF-LU}(A) \) or both rows and columns \( k-1 \) and \( k \) of \( \text{REF-LU}(A) \). The column permutation requires less effort and can be performed whenever \( u_{k-1,k} \neq 0 \); the row and column permutation can always be performed, since \( u_{k,k} = \rho^{(k)} \neq 0 \). Second, the effects of the permutation operation are propagated to the remainder of \( \text{REF-LU}(A) \) as well as to the working update vectors and factorization. The permutation may also require performing IPGE pivoting operations on the entry that will become the new \( k \)th pivot element of \( \text{REF-LU}(\hat{A}) \). The pseudocode of this adjustment subroutine is provided by Algorithm 3 in the Appendix (the pseudocode for the case with \( z_k^{(k-1)} = 0 \) is provided by Algorithm 4 therein). The proof of the ensuing theorem provides more details on how this adjustment is performed efficiently via roundoff error-free operations defined for LP-related updates in [Escobedo and Moreno-Centeno (2017)].

**Theorem 8.** The specified adjustments successfully overcome Special Cases 1 and 2 of the REF rank-one update, and their implementation keeps the algorithm to \( O(n^2) \) total operations.

**Proof.** For Special Case 1, we have that \( \hat{a}_{ij} = a_{ij} + v_i w_j = a_{ij} \) whenever \( v_i = 0 \) or \( w_i = 0 \), meaning that all entries along the first \( \theta_v \) rows and the first \( \theta_w \) columns of \( A \) and \( \hat{A} \) are identical. Accordingly, the entries of \( \text{REF-LU}(\hat{A}) \) along rows \([\theta_v] \) and columns \([\theta_w] \) match those of \( \text{REF-LU}(A) \) and can be copied directly. Hence, the algorithm can skip the calculations within its inner for-loop until it reaches the entries along row \( \theta_v+1 \) of \( \hat{U} \) or column \( \theta_w+1 \) of \( \hat{L} \). Because this adjustment can only decrease the number of inner-for-loop operations that must be performed by the algorithm, this special case requires \( O(n^2) \) total operations.

For Special Case 2, recall that subvectors \( A_{[k]}^1, A_{[k]}^2, \ldots, A_{[k]}^n \) are linearly independent, for all \( k \geq 1 \), based on Assumption 2 (if row and/or column permutations are required during the factorization of \( A \), these arguments would apply to the permuted matrix, say \( P_r A P_c \)). This also implies that subvectors \( A_{[i]}^1, A_{[i]}^2, \ldots, A_{[i]}^k \) are linearly independent, where \( k \leq i \leq n \). Next, it is useful to re-express \( y_k^{(k-1)} \) as:

\[
y_k^{(k-1)} = a_{k,n+1}^{(k-1)} = \det \left( A_{[k]}^{(k-1),n+1} \right),
\]

where the first equation is obtained from the properties of REF forward substitution and the second from the relationship between IPGE entries and the determinants of submatrices of \( A \) (see Equation 3). Based on this.
relationship, \( y_k^{(k-1)} = 0 \) implies that \( v_{[k]} \) is in the span of the linearly independent subvectors \( A_{[k]}^1, \ldots, A_{[k]}^{k-1} \), that is,

\[
\sum_{j=1}^{k-1} \alpha_j A_{[k]}^j = v_{[k]},
\]

for some \( \alpha_1, \ldots, \alpha_{k-1} \in \mathbb{R}^1 \). When this occurs, however, \( v_{[k]} \) cannot be simultaneously in the span of subvectors \( A_{[k]}^1, A_{[k]}^{k-2}, A_{[k]}^k \). We show this through contradiction by assuming that \( v_{[k]} \) can be expressed as:

\[
\sum_{j=1}^{k-2} \beta_j A_{[k]}^j + \beta_{k-1} A_{[k]}^k = v_{[k]},
\]

for some \( \beta_1, \ldots, \beta_{k-1} \in \mathbb{R}^1 \). Combining Equations (31) and (32) gives

\[
\sum_{j=1}^{k-2} \beta_j A_{[k]}^j + \beta_{k-1} A_{[k]}^k = \sum_{j=1}^{k-1} \alpha_j A_{[k]}^j
\]

\[
\beta_{k-1} A_{[k]}^k = \sum_{j=1}^{k-2} (\alpha_j - \beta_j) A_{[k]}^j + \alpha_{k-1} A_{[k]}^{k-1}
\]

\[
A_{[k]}^k = \sum_{j=1}^{k-2} \left( \frac{\alpha_j - \beta_j}{\beta_{k-1}} \right) A_{[k]}^j + \left( \frac{\alpha_{k-1}}{\beta_{k-1}} \right) A_{[k]}^{k-1}.
\]

The bottom equation indicates that subvector \( A_{[k]}^k \) is in the span of subvectors \( A_{[k]}^1, \ldots, A_{[k]}^{k-1} \), contradicting the assumption that subvectors \( A_{[k]}^1, \ldots, A_{[k]}^{k-1} \) are linearly independent. Therefore, \( v_{[k]} \) cannot also be in the span of subvectors \( A_{[k]}^1, A_{[k]}^{k-2}, A_{[k]}^k \). This implies that, if columns \( k-1 \) and \( k \) of REF-LU(\( A \)) are exchanged, the new value of \( y_k^{(k-1)} \)—equal to \( \det \left( A_{[k]}^{[k-2],n+1} \right) \)—must be nonzero. Through a similar line or reasoning, if both rows \( k-1 \) and \( k \) and columns \( k-1 \) and \( k \) of the original factorization are exchanged, the new value of \( y_k^{(k-1)} \) must be nonzero since

\[
\det \left( A_{[k]}^{[k-2],n+1} \right) = - \det \left( A_{[k]}^{[k-2],n+1} \right) \neq 0.
\]

In summary, when \( y_k^{(k-1)} = 0 \), permuting columns \( k-1 \) and \( k \) or both rows and columns \( k-1 \) and \( k \) of REF-LU(\( A \)) changes the value of \( y_k^{(k-1)} \) to be nonzero.

Finally, the adjustment for Special Case 2 can be performed efficiently and without roundoff error via an Adjacent Pivot Column Permutation or an Adjacent Pivot Diagonal Permutation of REF-LU(\( A \)), two operations originally defined in Escobedo and Moreno-Centeno (2017) for performing LP-related updates. Both subroutines are roundoff error-free and require \( O(n) \) operations. In the worst case, one of these two subroutines must be called in the initial steps of REF-ROU and prior to the start of each of its \( n-2 \) outer for-loop iterations—this occurs precisely when \( v \) is a multiple of \( A_{[k]}^1 \). However, because \( y_k^{(k-1)} \) is guaranteed to become non-zero after each call, this special case still requires \( O(n^2) \) total operations. \( \square \)

5. Computational Tests

This section presents two computational experiments on fully dense, randomly generated matrices \( A \in \mathbb{Z}^{n \times n} \), where \( n = 2^4, 2^5, \ldots, 2^{10} \). \( A \)'s entries are drawn uniformly from the non-zero integers in the interval \([-100,100]\).

The first experiment generates the update vectors \( v, w \in \mathbb{Z}^n \) randomly using the same specifications as the entries of \( A \). The second experiment copies a leading segment of \( v \) from a column of \( A \), and it generates
its remaining entries as in the first experiment. Specifically, a column index \( c \) is drawn uniformly from the integers in the interval \([1, n]\), and a row parameter \( r \) is drawn uniformly from the integers in the interval \([c, n]\); then the leading segment of \( v \) is set as \( v_{[c]} = A_{[c]} \), and the entries of its trailing segment \( v_{[n]\setminus[r]} \) are generated randomly. Based on the analysis from Section 4.3, this second way of generating \( v \) triggers at least \((r - c)\) calls to the Special Case 2 adjustment.

All experiments were carried out on a computer with an Intel(R) Xeon(R) CPU E5-2680 @ 2.40 GHz with 64 GB RAM. The code was written in C++ using the unlimited-precision GNU Multiple Precision Arithmetic Library (GMP). The experiments record the times required to compute the \( \text{REF LU} \) factorization of \( \hat{A} = A + vw^T \) from scratch and to obtain the factorization from an existing \( \text{REF LU} \) factorization of \( A \). The results are shown in Table 1 under columns “\( \text{REF-LU}(\hat{A}) \) (s)” and “\( \text{REF-ROU} \) (s)”, respectively. Therein, for each tested value of \( n \), the arithmetic mean and standard deviation of run-times over 30 different instances are reported in seconds (s), rounded to three decimals. For the second experiment, the table also reports summary statistics on the number of calls to the Special Case 2 adjustment (under column “\( \text{SC2-Calls} \)”), rounded to one decimal.

| \( n \) | \( \text{Run-times (s)} \) | \( \text{Run-times (s)} \) |
|---|---|---|
| | \( \text{REF-LU}(\hat{A}) \) | \( \text{REF-ROU} \) |
| | AVG | SD | AVG | SD |
| 16 | 0.000 | 0.000 | 0.000 | 0.000 |
| 32 | 0.001 | 0.000 | 0.000 | 0.000 |
| 64 | 0.015 | 0.003 | 0.004 | 0.001 |
| 128 | 0.161 | 0.015 | 0.019 | 0.002 |
| 256 | 2.484 | 0.016 | 0.150 | 0.001 |
| 512 | 57.061 | 1.652 | 1.554 | 0.048 |
| 1024 | 1357.219 | 17.664 | 17.763 | 0.114 |

| \( n \) | \( \text{Run-times (s)} \) | \( \text{Run-times (s)} \) | \( \text{SC-2 Calls} \) |
|---|---|---|---|
| | \( \text{REF-LU}(\hat{A}) \) | \( \text{REF-ROU} \) | AVG | SD |
| | AVG | SD | AVG | SD | AVG |
| 16 | 0.000 | 0.000 | 0.000 | 0.000 | 4.6 | 3.8 |
| 32 | 0.002 | 0.001 | 0.001 | 0.000 | 7.8 | 6.5 |
| 64 | 0.016 | 0.003 | 0.004 | 0.001 | 13.2 | 11.5 |
| 128 | 0.161 | 0.015 | 0.023 | 0.006 | 31.8 | 28.7 |
| 256 | 2.492 | 0.043 | 0.182 | 0.031 | 52.6 | 49.3 |
| 512 | 55.578 | 0.226 | 1.893 | 0.322 | 118.9 | 104.4 |
| 1024 | 1354.077 | 9.807 | 22.629 | 3.720 | 281.2 | 221.0 |

As expected, the results demonstrate that obtaining \( \text{REF-LU}(\hat{A}) \) by performing a \( \text{REF} \) rank-one update is orders of magnitude faster than constructing this \( \text{REF LU} \) factorization from scratch. In the first experiment, the exact update required less than 18 seconds while the refactorization required over 22 minutes, on average, for the largest matrix tested—which has over 1,000,000 non-zeros. Stated otherwise, the update could be performed close to 76-times in the time it takes to build the factorization for a matrix of this size. In the second experiment, this performance advantage decreased to 61-times, on account of the high number of calls to the \( \text{ACPU} \) algorithm that are needed to adjust for Special Case 2, based on the way that \( v \) is generated (i.e., we force \( y^{(k-1)}_b = 0 \) for a high number of iterations). Even with this extra effort, however, the average \( \text{REF-ROU} \) times are under 23 seconds. For completeness, Figure 1 plots the average of the performance ratios \( \text{REF-LU}(\hat{A})/\text{REF-ROU} \), for both experiments and all tested values of \( n \).
It is important to add that no calls to ACPU were required for any of the 210 instances tested in Experiment 1, indicating that it is highly unlikely for a leading segment of $v$ ($w$, resp.) to be linearly dependent on the corresponding segments of the first columns (rows, resp.) of $A$, when the input matrix and update vectors are fully dense and randomly generated as in the featured experiments.

![Figure 1](image_url)

**Figure 1** Run-time Ratios of Exact Factorization to the Rank-one Update Algorithm

6. Conclusion and Future Work

This work introduces a direct solution approach for efficiently solving systems of linear equations (SLEs) obtained from rank-one modifications, which are core subroutines used in nonlinear programming (NLP) and many other scientific applications. More specifically, it introduces algorithms for updating existing exact LU and Cholesky factorizations using integer-preserving arithmetic, rather than building new exact factorizations each time the current SLE is modified. The formal guarantees of the algorithms are formally established through the derivation of theoretical insights, and their computational advantages are supported with computational experiments, which demonstrate upwards of 75x-improvements over exact factorization run-times on fully dense matrices with over one million entries. Altogether, the exact rank-one updates serve as a foundation for enabling the implementation of the roundoff-error-free (REF) optimization framework, originally developed for linear programming, within other types of optimization problems. In the next steps of this research, the REF rank-one updates will be used to supplement quadratic programming solvers for use with relevant applications (e.g., direct optimal control ([Ferreau et al. 2014, Lee 2011]). We will also devote efforts to tailoring the REF rank-one updates to sparse Cholesky factorizations ([Davis and Hager 2001, 2005]) and to their recent applications (e.g., [Herholz and Alexa 2018], Herholz and Sorkine-Hornung 2020).

It is important to add that recently [Weber et al. 2019] introduced an iterative refinement technique that can be used to calculate high precision KKT solutions of convex and non-convex quadratic programming problems. However, the guarantees of this and other indirect solution approaches (e.g., [Gill and Wong 2015]) depend on certain technical assumptions regarding the conditioning of the inputs and, as such, are not fail-proof. Future work will explore how this iterative refinement technique and the REF rank-one update
algorithms could be used in complementary fashion, similar to the implementation of LP iterative refinement and exact LU factorization within the SoPlex solver (Gleixner et al. 2015, Wunderling 1996), which is part of the SCIP Optimization Suite (Gamrath et al. 2020).

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Appendix

This appendix presents the algorithm subroutines associated with Special Case 2 of the REF Rank-One Update Algorithm described in Section 4.3. Algorithm 3 provides the necessary steps for ensuring that \( y_{k-1}^{(k-1)} \neq 0 \), and Algorithm 4 provides the necessary steps for ensuring that \( z_{k-1}^{(k-1)} \neq 0 \), where \( 2 \leq k \leq n-1 \). The two subroutines are assumed to be embedded within Algorithm 2 specifically, they are executed prior to each call of the REF forward substitution algorithm. The first line of these algorithms serves to check whether the next iteration of the REF forward substitution algorithm will yield a zero divisor in the rank-one update algorithm—that is, if \( y_{k-1}^{(k-1)} = 0 \) and \( z_{k-1}^{(k-1)} = 0 \), respectively—without actually having to perform the iteration. When this will occur, the algorithms perform the requisite row and/or column permutations of REF-LU(\(A\)) via an Adjacent Pivot Column Permutation update (APCPU), an Adjacent Pivot Row Permutation update (APRPU), or an Adjacent Pivot Diagonal Permutation update (APDPU); these special updates are defined in Escobedo and Moreno-Centeno (2017). In addition, the corresponding permutations are performed on the update vectors and working factorization and, in the case of APCPU and APRPU, \( O(n) \) IPGE pivoting operations are performed on the entry that will become the new \( k \)th pivot element of REF-LU(\(\hat{A}\)).

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Algorithm 3: ROU Special Case 2 Subroutine for Avoiding $y_k^{(k-1)} = 0$

\begin{algorithmic}
\If {$\hat{l}_{k-1,k} - \hat{l}_{k,k-1} y_{k}^{(k-2)} = 0$}
\State \text{/* Permute columns $k-1,k$ of $A$ and $\hat{U}$ and elements $k-1,k$ of $w$ and $z^{(k-1)} */$
\State $A_{[n]}^{k-1} \leftrightarrow A_{[n]}^{k}$
\State $\hat{U}_{[n]}^{k-1} \leftrightarrow \hat{U}_{[n]}^{k}$
\State $w_{k-1} \leftrightarrow w_{k}$
\State $z_{k-1}^{k-1} \leftrightarrow z_{k}^{k-1}$
\If {$\hat{u}_{k-1,k} = 0$}
\State \text{/* Permute rows and columns $k-1,k$ of REF-LU($A$), rows $k-1,k$ of $A$ and $\hat{L}$ and elements $k-1,k$ of $v,y^{(k-1)} */$
\State REF-LU($A$) $\leftarrow$ APDPU(REF-LU($A$), $k-1 \leftrightarrow k$)
\State $A_{[n]}^{k-1} \leftrightarrow A_{[n]}^{k}$
\State $\hat{L}_{[n]}^{k-1} \leftrightarrow \hat{L}_{[n]}^{k}$
\State $v_{k-1} \leftrightarrow v_{k}$
\State $y_{k-1}^{k-1} \leftrightarrow y_{k}^{k-1}$
\Else
\State \text{/* Permute columns $k-1,k$ of REF-LU($A$) */$
\State REF-LU($A$) $\leftarrow$ APCPU(REF-LU($A$), $k-1 \leftrightarrow k$)
\State \text{/* Perform $k-2$ IPGE pivoting operations on the entry that will become the new $k$th pivot element of REF-LU($\hat{A}$) */$
\State $\hat{l}_{k,k} \leftarrow a_{k_k}^{(0)} v_{k} w_{k}$
\For { $i = 1, \ldots, k-2$}
\State $\hat{l}_{k,k} \leftarrow \hat{l}_{i} \hat{l}_{k,k} - \hat{u}_{i} \hat{a}_{k,i}$
\If {$i \geq 2$}
\State $\hat{u}_{k,k} \leftarrow \hat{l}_{k,k}/\hat{l}_{i-1,j-1}$
\EndIf
\EndFor
\EndIf
\EndIf
\EndIf
\EndAlgorithmic
Algorithm 4: ROU Special Case 2 Subroutine for Avoiding $z_k^{(k-1)} = 0$

if $\hat{u}_{k-1,k-1} z_k^{(k-2)} - \hat{u}_{k-1,k-1} z_k^{(k-2)} = 0$
   \* Permute rows $k-1,k$ of $A$ and $\hat{L}$ and elements $k-1,k$ of $v$ and $y^{(k-1)}$ *
   $A_{k-1}^{[n]} \leftrightarrow A_{k}^{[n]}$
   $\hat{f}_{k-1}^{[n]} \leftrightarrow \hat{f}_{k}^{[n]}$
   $v_{k-1} \leftrightarrow v_{k}$
   $y_{k-1}^{(k-1)} \leftrightarrow y_{k}^{(k-1)}$

if $\hat{l}_{k,k-1} = 0$
   \* Permute rows and columns $k-1,k$ of REF-LU($A$), columns $k-1,k$ of $A$ and $\hat{U}$ and elements $k-1,k$ of $w,z^{(k-1)}$ *
   REF-LU($A$) $\leftarrow$ APDPU(REF-LU($A$), $k-1 \leftrightarrow k$)
   $A_{k-1}^{[n]} \leftrightarrow A_{k}^{[n]}$
   $\hat{U}_{k-1}^{[n]} \leftrightarrow \hat{U}_{k}^{[n]}$
   $w_{k-1} \leftrightarrow w_{k}$
   $z_{k-1}^{(k-1)} \leftrightarrow z_{k}^{(k-1)}$

else
   \* Permute rows $k-1,k$ of REF-LU($A$) *
   REF-LU($A$) $\leftarrow$ APRPU(REF-LU($A$), $k-1 \leftrightarrow k$)
   \* Perform $k-2$ IPGE pivoting operations on the entry that will become the new $k$th pivot element of REF-LU($\hat{A}$) *
   $\hat{l}_{k,k} \leftarrow a_{k,k}^{(0)} + v_{k} w_{k}$
   for $i = 1, \ldots, k-2$ do
      $\hat{l}_{k,k} \leftarrow \hat{l}_{i,k} \hat{l}_{k,i} - \hat{u}_{i,k} \hat{l}_{k,i}$
      if $i \geq 2$
         $\hat{l}_{k,k} \leftarrow \hat{l}_{k,k} / \hat{l}_{i-1,i-1}$
      $\hat{u}_{k,k} \leftarrow \hat{l}_{k,k}$

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