Applications of the Gauss-Jordan algorithm, done right

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January 27, 2014

Abstract

Computer Algebra systems are widely spread because of some of their remarkable features such as their ease of use and performance. Nonetheless, this focus on performance sometimes leads to unwanted consequences: algorithms and computations are implemented and carried out in a way which is sometimes not transparent to the users, and that can lead to unexpected failures. In this paper we present a formalisation in a proof assistant system of a naive version of the Gauss-Jordan algorithm, with explicit proofs of some of its applications, and additionally a process to obtain versions of this algorithm in two different functional languages (SML and Haskell) by means of code generation techniques from the verified algorithm. The obtained programs are then applied to test cases, which, despite the simplicity of the original algorithm, have shown remarkable features in comparison to some Computer Algebra systems, such as Mathematica® (where some of these computations are even incorrect), or Sage (in comparison to which the generated programs show a compelling performance). The aim of the paper is to show that, with the current technology in Theorem Proving, formalising Linear Algebra procedures is a challenging but rewarding task, which provides programs that can be compared in some aspects to state of the art procedures in Computer Algebra systems, and whose correctness is formally proved.

Index terms — Numerical Linear Algebra, Algorithm implementation, Isabelle/HOL, Code generation

1 Introduction

Computer Algebra systems are used nowadays in very different environments and, after years of continuous improvement, with an ever increasing level of confidence. Despite this, these systems focus intensively on performance, and their
algorithms are subject to continuous refinements and modifications, which can sometimes derive in a loss of accuracy and even sometimes of correctness. On the other hand, theorem provers are designed to prove the correctness of program specifications and mathematical results. This task is far from trivial, and it does not pay off in terms of performance but only in terms of the simplicity and the insight of the programs one is trying to formalise. Consequently, one can be faced with the very little appealing situation where a program has been formalised but its usefulness is, at least, arguable.

Fortunately, and after years of continuous work, theorem proving tools have reduced this well-known gap, and the technology they offer is being used to implement and also to analyse state of the art algorithms and programs (see for instance [7, 19]). In this work, we present an experiment to formalise a version of the Gauss-Jordan algorithm over matrices in the theorem prover Isabelle/HOL. The algorithm computes the reduced row echelon form of a matrix, which is then proved to be applicable to solve standard problems in Linear Algebra, such as computing the rank of a linear form, computing determinants and inverses, solving systems of linear equations, and computing bases of fundamental subspaces of linear forms. These verified algorithms are later code-generated to the functional languages SML and Haskell. The code obtained in these languages is tested against a battery of examples. The algorithm that we implement is neither specialised, nor obtained from a Computer Algebra system, but just a simple version of the Gauss-Jordan algorithm. Nevertheless, the utility of our work is threefold. First, it shows that the formalisation of Linear Algebra algorithms in a theorem prover is feasible. Second, the code obtained in Haskell and SML, even if it lacks of the performance of the specialised code of standard Computer Algebra systems, was capable of computing some determinants with big integers that produced a bug in Mathematica® [6]. Finally, the already existing infrastructure in the Isabelle/HOL Multivariate Analysis Library allowed us to keep the ties among Linear Algebra algorithms and their mathematical meaning or origin (a feature that is not possible in Computer Algebra systems).

The paper will be divided as follows: in Section 2 we introduce the Isabelle/HOL theorem prover and the infrastructure in such system that is used in our work; we distinguish among the parts which are already in the system, and the ones that are product of our own work. In Section 3 we present a version of the Gauss-Jordan algorithm over fields, as well as the different applications of it that we have formalised in Isabelle/HOL. In Section 4 we present the code generation process from the formalised Isabelle algorithm to the running versions in SML and Haskell. Finally, in Section 6 we draw some conclusions and possible research lines that follow from our work.

The source files of the development are available from [5]: they have been developed under the Isabelle 2013-2 version. The previous web site also includes the SML and Haskell code generated from the Isabelle specifications, and also the input matrices that have been used in the benchmarks presented in Section 5.
2 Isabelle

2.1 Isabelle/HOL

Isabelle [17] is a generic theorem prover which has been instantiated to support different object-logics, from which higher-order logic (or briefly, HOL [16]) is the one that offers a greatest number of facilities to the user, some of which will be relevant to our work (such as code generation [23]). The Isabelle metalogic is based on two components: a (rather simple) type system, including non-empty types and function types ($\alpha \to \beta$), from which the $\text{prop}$ type includes the propositions accepted by the system, and a set of inference rules acting over elements of $\text{prop}$ type, expressing the properties of the metalogic connectors (implication, universal quantifier and logical equivalence). New propositions in the system are then elements of type $\text{prop}$ that, by means of iterative applications of inference rules, have been reduced to trivial propositions (the $\text{True}$ constant).

From the previous simple infrastructure, Isabelle/HOL introduces then some new connectors (specialised versions of the metalogic ones for this particular logic) and additional axioms (such as for instance the law of excluded middle). We briefly present here the features of Isabelle/HOL in which our work relies on. The previous references offer further insight.

The HOL type system is based on non-empty types, function types ($\Rightarrow$) and type constructors $\kappa$ that can be applied to already existing types ($\text{nat}$, $\text{bool}$) or type variables ($\alpha$, $\beta$). Types can be also introduced by enumeration ($\text{bool}$) or by induction, as lists (by means of the $\text{datatype}$ command). Additionally, new types can be also defined as non-empty subsets of already existing types ($\alpha$) by means of the $\text{typedef}$ command; the command takes a set defined by comprehension over a given type $\{x :: \alpha. P\ x\}$, and defines a new type $\sigma$.

Isabelle also introduces type classes in a similar fashion to Haskell; a type class is defined by a collection of operators (over a single type variable) and premises over them. For instance, the HOL Multivariate Analysis library has a type class $\text{field}$ representing the algebraic structure. Concrete types ($\text{real}$, $\text{rat}$) can be proven to be instances of a given type class ($\text{field}$ in our example). Type classes are also used to impose additional restrictions over type variables; for instance, the expression ($x :: \alpha :: \text{field}$) imposes the constraint that the type variable $\alpha$ possess the structure and properties stated in the $\text{field}$ type class, and can be later replaced exclusively by types which are instances of that type class.

2.2 HOL Multivariate Analysis

The HOL Multivariate Analysis (or $\text{HMA}$ for short) Library is a set of Isabelle theories which contains a number of theoretical results in mathematical fields such as Analysis, Topology or Linear Algebra. They are based on previous work of J. Harrison in HOL-Light [9], which includes proofs of intricate theorems (such as the Stone-Weierstrass theorem) and has been used as a basis for appealing projects such as the formalisation of the proof of the Kepler conjecture by T. Hales. Among the fundamentals of the library, one of the keys is the representation of $n$-dimensional vectors over a given type ($\mathbb{F}^n$, where $\mathbb{F}$ stands for a generic field, or in Isabelle jargon a type variable $\alpha :: \text{field}$).

The idea is to represent vectors over $\alpha$ by means of functions from a finite
type variable \( \beta :: \text{finite} \) to \( \alpha \); for proving purposes, this type definition is usually sufficient to support the generic structure \( \mathbb{R}^n \).

The Isabelle type definition is as follows; the functions \( \text{vec-nth} \) and \( \text{vec-lambda} \) are the morphisms between the abstract data type \( \text{vec} \) and the underlying concrete data type, functions with finite domain (the mathematical restrictions over \( \alpha \) and \( \beta \) are added only when required for formalisation purposes):

\[
\text{typedef} \ (\alpha, \beta) \ \text{vec} = \text{UNIV} :: (\beta::\text{finite}) \Rightarrow \alpha \ \text{set}
\]

\[
\text{morphisms} \ \text{vec-nth} \ \text{vec-lambda} ..
\]

The previous type also admits in Isabelle the shorter notation \( \alpha \hat{\beta} \). The idea of using underlying finite types for vectors indices has great advantages, as already pointed out by Harrison, from the formalisation point of view. For instance, the type system enforces that operations on vectors (such as addition or multiplication) are only performed over vectors of equal dimension, i.e., vectors whose indexing types are exactly the same (this would not be the case if we were to use, for instance, lists as vectors). Moreover, the functional flavour of operations and properties over vectors is kept (for instance, vector addition can be defined in a pointwise manner).

The representation of matrices is then derived in a natural way based on the one of vectors by iterating the previous construction (matrices over a type \( \alpha \) will be terms of type \( \alpha \hat{m} \hat{n} \), where \( m \) and \( n \) stand for finite type variables).

A subject that has been explored neither in the Isabelle HMA Library, nor in HOL-Light, is the possibility to execute the previous data types and operations. Another aspect that has not been explored in the HMA Library is Numerical Linear Algebra. One of the novelties of our work is to establish a link between this formalisation setting and a framework where algorithms can be represented and also executed.

### 2.3 Code generation

Another interesting feature of Isabelle/HOL is its code generation facility \cite{10}. Its starting point are specifications (in the form of the different kinds of definitions supported by the system) whose properties can be stated and proved, and (formalised) rewriting rules that express properties from the original specifications. From the previous code equations, a shallow embedding from Isabelle/HOL to an abstract intermediate functional language (Mini-Haskell) is performed. Finally, trivial transformations to the functional languages SML, Haskell, Scala and OCaml are performed. The expressiveness of HOL (such as for instance universal or existential quantifiers, or the Hilbert’s \( \epsilon \) operator) is not that of functional programming languages, and therefore one must restrict herself to use Isabelle “executable” specifications, if she aims at generating code from them (or prove code equations that refine non-executable specifications to executable ones).

The generated code satisfies a principle of partial correctness by construction, with respect to the properties that have been proved of it. This means that whenever an expression \( v \) is evaluated to some term \( t \), \( t = v \) is derivable in the equational semantics of the intermediate language. See \cite{12,9} for further details.
3 The Gauss-Jordan algorithm and its applications

In a previous work [2], we formalised the rank plus nullity theorem of Linear Algebra. In our proof it is established that, given \( V \) a finite-dimensional vector space over \( \mathbb{R} \), \( W \) a vector space over \( \mathbb{R} \), and \( \tau \in L(V, W) \) (a linear form between \( V \) and \( W \)), \( \dim(\ker(\tau)) + \dim(\text{im}(\tau)) = \dim(V) \) or, in other notation, \( \text{null}(\tau) + \text{rk}(\tau) = \dim(V) \). We closely followed the proof in [8], as we follow here his notation. Unfortunately, having formalised the previous result does not provide us with an algorithm computing the dimension of the image and kernel sets of a given linear form.

As it has been proved in the HMA Library, every linear form between finite-dimensional vector spaces over the field \( \mathbb{R} \) is equivalent to a matrix over \( \mathbb{R}^{m \times n} \), and therefore we can reduce the computation of the dimensions of the range (or rank) and the kernel (or nullity) of a linear form to the computation of the reduced row echelon form [18] (or \text{rref}) of a matrix; the number of nonzero rows of such matrix provides its rank, and the number of zero rows its nullity. The Gauss-Jordan algorithm computes the \text{rref} of a matrix.

We have formalised in Isabelle the following version of the Gauss-Jordan algorithm:

\begin{algorithm}
\begin{algorithmic}
\State \textbf{Data:} \( A \) is the input matrix; \hspace{1cm} \triangleright \ l \text{ is the index where the pivot is placed}
\State \( l \leftarrow 0; \)
\For {\( k \leftarrow 0, (\text{ncols}\ A) - 1 \)} \hspace{1cm} \triangleright \text{Check that col.} \ k \text{ contains a pivot over index} \ l
\If {\text{nonzero} \ l(\text{col}\ A \ k)} \hspace{1cm} \triangleright \text{Let} \ i \text{ be the index of first nonzero entry over} \ l
\State \( i \leftarrow \text{index-nonzero} \ l(\text{col}\ A \ k) \) \hspace{1cm} \triangleright \text{Rows} \ i \text{ and} \ l \text{ are interchanged}
\State \( A \leftarrow \text{interchange-rows} \ A \ i \ l \) \hspace{1cm} \triangleright \text{Row} \ l \text{ is multiplied by} \ (1/A \ l \ k)\)
\State \( A \ l \leftarrow \text{mult-row} \ A \ l \ (1/A \ l \ k) \)
\For {\( t \leftarrow 0, (\text{nrows}\ A) - 1 \)} \hspace{1cm} \triangleright \text{Row} \ t \text{ is added row} \ l \text{ times} \ (-A \ t \ k)\)
\If {\( t \neq l \)} \hspace{1cm} \triangleright \text{Row} \ t \text{ is added row} \ l \text{ times} \ (-A \ t \ k)\)
\State \( A \ t \leftarrow \text{add-row} \ A \ t \ l \ (-A \ t \ k) \)
\EndIf
\EndFor
\State \( l \leftarrow l + 1 \)
\EndIf
\EndFor
\end{algorithmic}
\end{algorithm}

The algorithm traverses the columns of the input matrix, finding in each column \( k \) a pivot \( i \) (the first nonzero element in a row greater than index \( l \)); if the pivot exists, rows \( i \) and \( l \) are interchanged (if the matrix has maximum rank, \( l \) will be equal to the column index, otherwise it will be smaller), and row \( l \) is multiplied by the inverse of the pivoted element; this row is used to perform row
operations to reduce all remaining coefficients in column \( k \) to 0. If a column does not contain a pivot, the algorithm processes the next column. The algorithm performs exclusively elementary row operations. We have expressed it above with imperative constructs such as for and variable assignments that are not native to the Isabelle/HOL specification language. In our Isabelle specification, rows and columns are assigned finite enumerable types, over which matrices are represented as functions. The previous algorithm operations are expressed by means of functions representing the output matrix after each operation. Note that a matrix is defined by means of a function over the rows type of functions over the columns type. For instance, the Isabelle definition shown below is the one selecting a pivot \( i \) in column \( k \) over the index \( l \) (line 5 in Algorithm 1), interchanging rows \( i \) and \( l \) (line 6), multiplying the row \( l \) by the multiplicative inverse of \( A[l,k] \) (line 7) and reducing the rest of the rows of the matrix, by means of a lambda expression, which represents the new created matrix (lines 8 to 12).

The traversing operation over columns (line 3) is represented by means of a fold operation over the list containing the columns type universe.

\[
\text{Gauss-Jordan-in-pos \, A \, l \, k =} \\
\text{(let)} \\
\quad i = (\text{LEAST } n. A[n,k] \neq 0 \land n \geq l); \\
\quad \text{interchange}_A = (\text{interchange}_\text{rows} \ A \ i \ l); \\
\quad A' = \text{mult}_\text{row} \ \text{interchange}_A \ l \ (1/\text{interchange}_A[l][k]) \\
\quad \text{in} \\
\quad \text{vec}_\lambda(\lambda t. \text{if } t=l \text{ then } A'[l] \ \text{else } (\text{row}_\text{add} \ A' \ t \ l \ (-\text{interchange}_A[l][k]))) \\
\]

The algorithm has several variants, both to speed up its performance and also to avoid numerical stability issues with floating point numbers [8, Ch. 9], but in order to reduce the complexity of its formalisation we chose the presented one. As we show later (Section 5) its performance is noticeable.

The \text{rref} of a matrix has indeed further applications than computing the rank; based on the fact that the version of Gauss-Jordan used to obtain it is based on elementary row operations, it can be also used for the following ends:

- Computation of the inverse of a matrix, by “storing” the elementary row operations over the identity matrix.
- Determinants, taking into account that some of the elementary row operations can introduce multiplicative constants.
- Computation of bases and dimensions of the null (defined as \( \{x \in \mathbb{R}^n \mid A \ast x = 0\} \)), left null (\( \{x \in \mathbb{R}^n \mid x^T \ast A = 0\} \)), column (\( \{A \ast x \mid x \in \mathbb{R}^n\} \)) and row (\( \{A^T \ast x \mid x \in \mathbb{R}^n\} \)) subspaces of a matrix.
- Solutions of systems of linear equations (\( \{x \mid A \ast x = b \land x \in \mathbb{R}^n\} \)), both consistent (with unique or multiple solutions) and inconsistent ones.

The formalisation of the Gauss-Jordan algorithm and the different applications that are presented above summed up 8000 lines of code; the proofs are devoted to check that the defined objects (determinant, inverse matrix, solution of the linear system) are preserved (or modified in a certain way) after each algorithm step (and more concretely, after each row operation). By using product
types, we store the input matrix and we set an initial value for the defined object. In the case of determinants, the initial pair is \((1_n, A)\). The other computations start from \((I_n, A)\) or \((I_m, A^T)\). After each algorithm step, the corresponding modification is applied to the first component. In the computation of each of the previous pairs, there is a notion of invariant that is preserved through the Gauss-Jordan algorithm steps. For instance, in the case of determinants, given a matrix \(A\), after \(n\) elementary operations the pair \((b_n, A_n)\) is obtained, and it holds that \(\det A = b_n \ast (\det A_n)\). Since the algorithm is terminating (the elements indexing the columns are an enumerable type), after a finite number \(m\) of operations we obtain a pair \((b_m, \text{rref}A)\) such that \(\det A = b_m \ast (\det(\text{rref}A))\); since we proved that the determinant of \(\text{rref}A\) is the product of its diagonal elements, the computation is completed.

In a similar way we perform the proof of the computation of the inverse of a matrix (starting from an input square matrix \(A\) of dimension \(n\), the pair \((I_n, A)\) is built and after every row operation, \((P', A')\) is such that \(P' \ast A = A'\), as long as \(A\) is invertible (in other words, \(\text{rref}A = I_n\)). When the Gauss-Jordan algorithm reaches \(\text{rref}A\), the first component of the pair holds the matrix \(P\), which is the product of every elementary operation performed. The computation of the bases of the fundamental subspaces of linear forms are also based on the computation of the matrix \(P\) generated from applying the Gauss-Jordan algorithm to \(A\) (or \(A^T\)) and the same operations to \(I_n\) (or \(I_m\)). Their Isabelle definitions follow:

```isabelle
definition basis_null_space A = 
  {row i (P_Gauss_Jordan (transpose A)) | i. to_nat i ≥ rank A}
definition basis_row_space A = {row i (Gauss_Jordan A) | i. row i (Gauss_Jordan A) ≠ 0}
definition basis_col_space A = 
  {row i (Gauss_Jordan (transpose A)) | i. row i (Gauss_Jordan (transpose A)) ≠ 0}
definition basis_left_null_space A = 
  {row i (P_Gauss_Jordan A) \ i. to_nat i ≥ rank A}
```

With respect to the solution of systems of linear equations \(A \ast x = b\), we prove that, if a system is consistent, its set of solutions is equal to a single point plus any element which is solution to the homogeneous system associated to the input system of equations, \(A \ast x = 0\) (or, in other words, the null space of \(A\)). We also prove that every solution of the system must be of this form. Therefore, in order to solve a system, we start from the pair \((I_n, A)\) and after applying the Gauss-Jordan algorithm to the second component, and the same elementary operations to the first component, \((P, \text{rref}A)\) is obtained. The vector \(b\) is multiplied by the matrix \(P\), and from its number of nonzero positions and the rank of \(A\) (or \(\text{rref}A\)) the system is classified as consistent or inconsistent. In the first case, a single solution is computed by taking advantage of \(\text{rref}A\). The basis of the null space is computed applying Gauss-Jordan elimination to \(A^T\) in \((I_m, A^T)\), and performing similar row operations to \(I_m\).

In order to consider inconsistent systems suitably, we have represented the solutions as elements of the Isabelle option type \((\text{SOME} x. P x), \text{NONE}\), which are presented as a singular point (whenever the system has solution), and the corresponding vectors forming a basis of the null space (or the empty set).
We have formalised in Isabelle that every solution to a given system is of the previous form (most Computer Algebra systems, and previous formalisations of the solution of systems of linear equations through Gauss-Jordan algorithm \cite{15} compute single solutions and sometimes for exclusively compatible systems with equal number of equations and unknowns).

Regarding the complexity, Gauss-Jordan algorithm is well-known to perform $O(n^3)$ operations for input square matrices of dimension $n \times n$. The amount of operations involved in the computation of the rref, the rank, the determinant and the row and column spaces, following our ideas, will be of such order (except for the computation of the transpose). In order to compute the inverse of a matrix, the number of columns double, but the number of rows is preserved; the arithmetic operations are twice the number of operations performed in the rref. The same number of operations are performed for the computation of the null and left null spaces, since they require computing the $P$ matrix associated to rref $A$. Finally, computing the solutions of a system of linear equations involves the computation of the rref of $A$ and its $P$ matrix, and also the computation of the rref of $A^T$ and its corresponding $P$ matrix.

### 4 Code generation to functional languages

The previous version of the Gauss-Jordan algorithm can be directly executed inside of Isabelle (by rewriting specifications and code equations) with some setup modifications that we presented in a previous work \cite[Sec. 4]{3}. The specifications are themselves executable, since we are dealing with finite types for representing matrices columns and rows. For instance, the Isabelle function Gauss-Jordan-in-pos presented above, that makes use of the \texttt{LEAST} operator (based itself on the Hilbert’s $\epsilon$ operator), which is not executable in general, takes advantage of the fact that its underlying type is enumerable, and can be executed to select a pivot. Unfortunately, the performance obtained makes the algorithm unusable in practice, except for testing small examples. Matrices represented as functions over finite domains are reportedly impractical. More concretely, there are two sources of inefficiency in the results obtained. First, Isabelle is not designed as a programming language, and execution inside of the system offers a not remarkable performance. In Section 4.1 we present a solution to translate our specifications to functional programming languages. Second, the data structures (functions) that helped us to prove the correctness of the Gauss-Jordan algorithm and its applications are optimal for formalisation, but not for execution. Section 4.2 describes a verified refinement between the type used for representing matrices in our formalisation ($\texttt{vec}$ and its iterated construction) and \texttt{immutable arrays}, a common data structure in functional programming.

#### 4.1 Code generation and serialisations

The first problem is solved by generating our specifications to a programming (functional) language, as introduced in Section 2.3. Our choices (from the available languages in the standard Isabelle code generation setup) were SML (since the SML Standard Library includes a \texttt{Vector} type representing immutable arrays) and Haskell (for a similar reason, with the Haskell \texttt{IArray} class type and its corresponding instance \texttt{IArray..Array}, and also because it has a type $\texttt{Rational}$
representing arbitrary precision rational numbers).

Additionally, we make use of serialisations, a process to map Isabelle types and operations to corresponding ones in the target languages. Serialisations are common practice in code generation processes (see [10] for some introductory examples); otherwise, the source types and operations would be generated from scratch in the target languages, and the obtained code would be less usable and efficient (for instance, nat type would be generated to an ad-hoc type with 0 and Suc as constructors, and then int as the equivalence classes of pairs of naturals). The following Isabelle code snippet presents the serialisation that we produced from the Isabelle type rat representing rational numbers (which is indeed based on equivalence classes), to the Haskell type Rational. As it can be observed, it identifies operations (including type constructors) from the source and the target languages.

```
code_printing
  type_constructor rat ⇀ (Haskell) "Prelude.Rational"
  class_instance rat :: "HOL.equal" ⇒ (Haskell) -
  constant "0 :: rat" ⇀
    (Haskell) "Prelude.toRational (0::Integer)"
  constant "1 :: rat" ⇀
    (Haskell) "Prelude.toRational (1::Integer)"
  constant "Frct" ⇀
    (Haskell) "((let (x,y) = _ in (Rational.fract
      (integer'_of'_int x) (integer'_of'_int y)))"
  constant "quotient_of" ⇀
    (Haskell) "((let x = _ in
      (Int'_of'_integer (Rational.numerator x),
      Int'_of'_integer (Rational.denominator x)))"
  constant "HOL.equal :: rat ⇒ rat ⇒ bool" ⇀
    (Haskell) "(_ == (_)"
  constant "op < :: rat ⇒ rat ⇒ bool" ⇀
    (Haskell) "_ < _"
  constant "op ≤ :: rat ⇒ rat ⇒ bool" ⇀
    (Haskell) "_ <= _"
  constant "op + :: rat ⇒ rat ⇒ rat" ⇀
    (Haskell) "(_ + (_)"
  constant "op - :: rat ⇒ rat ⇒ rat" ⇀
    (Haskell) "(_ - (_)"
  constant "op * :: rat ⇒ rat ⇒ rat" ⇀
    (Haskell) "(_ * (_)"
  constant "op / :: rat ⇒ rat ⇒ rat" ⇀
    (Haskell) "(_ / (_)"
  constant "uminus :: rat ⇒ rat" ⇀
    (Haskell) "Prelude.negate"
```

The complete set of Isabelle serialisations that we have taken advantage of are shown in Table 1. The Isabelle types rat, real and bit represent respectively \( \mathbb{Q} \), \( \mathbb{R} \) and \( \mathbb{Z}_2 \). The SML type IntInf.int represents arbitrary precision integers. It is worth noting that the Isabelle type real can be also serialised to the ones used for rat in SML and Haskell, preserving arbitrary precision and avoiding numerical stability issues. Types presented in bold face identify serialisations that were introduced by us as part of this work. We also contributed some
improvements to the Isabelle Library in the serialisation to the SML type \textit{Vector}.

The SML Standard Library lacks of a type representing arbitrary precision rational numbers, and thus the proposed serialisation for \textit{rat} is quotients of arbitrary precision integers. As we will see in our performance tests (see Section 5) Haskell will take advantage of its native \textit{Rational} type to outperform SML. We explored the possibilities of double-precision floating-point formats (\textit{Double} in Haskell, \textit{Real.real} in SML) in the target languages in the search for a wider comparison of our algorithm with Computer Algebra systems. The \textit{bit} type admits multiple serialisations, ranging from boolean values to subsets of the integers. Experimental results showed us that the better performing option was to serialise \textit{bit} and its operations to integers in the target language and operations \textit{modulo} 2.

### 4.2 Data type refinements

Some data types present better properties for specification and formalisation purposes. For instance, specifying an algorithm over sets is easier than doing so over lists. However, the latter data type is better suited for execution tests. Following this idea, the poor performance presented by functions representing matrices can be solved by means of a data refinement to a better performing data structure.

Data refinement \cite{11} offers the possibility to replace an abstract data type in an algorithm by a concrete one; more concretely, our intention is to replace the \textit{vec} type representing vectors by means of a better performing type in the code generation process. In our development, we have used the Isabelle type \textit{iarray} as the target type of our refinement. Accordingly, we define functions \textit{vec-to-iarray} (and \textit{matrix-to-iarray}) that convert elements of type \textit{vec} to elements of type \textit{iarray}.

**definition** \textit{vec-to-iarray}::\texttt{''a''n::{mod_type}} ⇒ \texttt{''a iarray}

\textit{where} \texttt{vec-to-iarray A = IArray.of_fun (λi. A$(\texttt{from_nat i})) (\texttt{CARD('n))}}

Each function over elements of type \textit{vec} needs to be replaced by a new function over type \textit{iarray}. This requires first specifying a function over the type \textit{iarray}, and then proving that it behaves as the one over type \textit{vec}.

**lemma** \texttt{[code_unfold]}:

\textit{shows matrix-to-iarray} \texttt{(Gauss_Jordan A) = Gauss_Jordan_iarrays (matrix-to-iarray A)}

The previous lemma certifies that replacing the function \textit{Gauss-Jordan} (de-
fined over abstract matrices, or elements of type vec) by Gauss-Jordan-arrays is correct. As it can be observed, the lemma does not include premises; lemmas including premises cannot be used to get code generation, since premises could not be checked in the target languages. The label code-unfold instructs the code generation tool to record the lemma as a rewriting rule, replacing occurrences of the left-hand side in the execution and code generation processes by the right-hand side. From a more general perspective, the function matrix-to-array has to be proved to be a homomorphism between the original and the refined type.

The proving effort (in lines of code) to complete this task is almost as challenging as the one devoted to complete the formalisation of the original algorithm (6000 code lines). In our case, we preserved the original algorithm (we simply replace operations over the abstract type by equivalent ones over the concrete one) but Isabelle code generator leaves the door open to algorithmic refinements (obviously, when the differences between the original and the final algorithms are greater, the proving effort to fill such a gap will be more intense).

5 Performance of the generated programs

Once the previous serialisations have been completed, and going through the data type refinements presented in Section 4, our original specification of the Gauss-Jordan algorithm and the different applications presented in Section 3 are code generated to both SML and Haskell. The automatically generated code sums up 2,500 lines in SML and 2,400 in Haskell.

For the execution tests, we use the Poly/ML interpreter (version 5.5.1), the MLton optimizer compiler (version 20100608), and also the Haskell compiler GHC (version 7.4.1). We also include the Sage Mathematical Software System (5.13) in the comparison to establish a link between our performance results and the ones of a “real” system, even if we have not explored the algorithms implemented in Sage. In the tests about determinants, we also comment on a bug in Mathematica® 8.0, 9.0 and 9.0.1.

The tests have been carried out in a personal computer with an Intel® Icore™ i5-3360M processor (up to 2.8 GHz, 2 cores with 4 threads) with 4GB RAM memory.

Some preliminary experiments had been already carried out in MLton and Poly/ML, exclusively for the computation of the rank of linear forms [4], but developers of both tools suggested us improvements in our methodology that eliminated the processing time of the input matrices (which in MLton showed to be the real bottleneck, and also in Poly/ML a great waste of time, see the figures in [4]). In our first experiments, the input matrices, of size up to 2,560×2,560 were directly introduced in the system by means of an explicit binder, using the SML val command, as static data. At least in MLton, an intermediate type checker was getting extremely slow with input data of considerable size. The Poly/ML maintainer also modified the system behaviour in the SVN version of the tool (and now in the 5.5.1 stable version) to improve the processing capabilities of big inputs. From our side, we changed our methodology to input matrices from external files by means of an ad-hoc parser. Processing input matrices this way (at least, up to sizes of 2,560×2,560) proved to be no time consuming.

We present here a fragment of the experiments carried out with the new methodology. We completed experiments of the different applications of the
Table 2: Elapsed time (in seconds) to compute the rref of randomly generated $\mathbb{Z}_2^{n \times n}$ matrices.

| Size (n) | Poly/ML | MLton | Haskell | Sage |
|----------|---------|-------|---------|------|
| 100      | 0.04    | 0.06  | 6.26    | 0.04 |
| 200      | 0.25    | 0.46  | 49.24   | 0.04 |
| 300      | 0.85    | 1.52  | 170.39  | 0.04 |
| 400      | 2.01    | 3.52  | -       | 0.04 |
| 500      | 3.90    | 6.87  | -       | 0.04 |
| 600      | 6.16    | 11.77 | -       | 0.04 |
| 800      | 15.96   | 27.98 | -       | 0.04 |
| 1000     | 32.08   | 54.65 | -       | 0.04 |
| 1200     | 62.33   | 94.25 | -       | 0.05 |
| 1400     | 97.16   | 152.06| -       | 0.05 |
| 1600     | 139.70  | 225.76| -       | 0.05 |
| 1800     | 203.10  | 323.84| -       | 0.05 |
| 2000     | 284.28  | 437.35| -       | 0.05 |

Gauss-Jordan algorithm presented in Section 3 in the fields $\mathbb{Z}_2$, $\mathbb{Q}$ and $\mathbb{R}$.

Table 2 presents the results of computing the rref of $\mathbb{Z}_2$ matrices. As it can be noticed, Sage greatly outperforms our programs. The computing times of our programs grow linearly compared to the number of elements in the input matrices. It is noticeable that Poly/ML, which is an interpreter, performs better than an optimiser compiler as MLton. Haskell seems to run poorly when the number of elements grows.

Interestingly, the rank (the number of nonzero rows of the rref) of $\mathbb{Z}_2$ matrices permits the computation of the number of connected components of a digital image [13]; in Neurobiology, this technique can be used to compute the number of synapses in a neuron (see [4]). With our programs, the computations can be carried out on images of $2560 \times 2560$ px. (which are conventional sizes in real life experiments). The algorithm performs better with these matrices than with randomly generated ones (as the ones used in these tests).

Table 3 presents the performance tests to compute determinants of matrices over $\mathbb{Q}$. Apparently, Haskell takes advantage of its native Rational type to get better results than Poly/ML and MLton. Sage seems to require more time than for the rank computations with elements of type $\mathbb{Z}_2$.

The case of determinants of rational (or integer) matrices is specially interesting. Varona et al [6] detected that Mathematica®, in its versions 8.0, 9.0 and 9.0.1, was computing erroneously determinants of matrices of big integers, even for small dimensions (in their work they present an example of a matrix of dimension $14 \times 14$). The situation is such that even the same determinant, computed twice, produces two different results. The bug was reported to the Mathematica® support service. The error might be originated in the use of some arithmetic operations module large primes (that could be either not large enough, or not as many as required). With our verified program, the computation takes ca. 5 seconds (in Haskell; Poly/ML and MLton are slower, but also reach the same result), and the result obtained is the same as in Sage (which again requires 0.0 seconds) and Maple™. Our algorithm relies on the arbitrary precision integer numbers used in each one of the functional languages used, but
Table 3: Elapsed time (in seconds) to compute the determinant of randomly generated $\mathbb{Q}$ matrices.

| Size (n) | Poly/ML | MLton | Haskell | Sage |
|---------|---------|-------|---------|------|
| 10      | 0.02    | 0.01  | 0.06    | 0.00 |
| 20      | 0.35    | 0.10  | 0.12    | 0.00 |
| 30      | 1.92    | 0.61  | 0.51    | 0.00 |
| 40      | 6.70    | 2.17  | 1.60    | 0.01 |
| 50      | 20.26   | 6.73  | 4.34    | 0.01 |
| 60      | 43.02   | 14.38 | 8.86    | 0.02 |
| 70      | 87.20   | 29.20 | 17.16   | 0.03 |
| 80      | 155.14  | 51.56 | 29.81   | 0.04 |
| 90      | 263.60  | 88.15 | 49.22   | 0.05 |
| 100     | 425.75  | 142.38| 74.23   | 0.11 |

Table 4: Elapsed time (in seconds) to compute the inverse of randomly generated $\mathbb{R}^{n \times n}$ matrices.

| Size (n) | Poly/ML | MLton | Haskell | Sage |
|---------|---------|-------|---------|------|
| 100     | 0.08    | 0.09  | 10.36   | 0.05 |
| 200     | 0.57    | 0.65  | 82.10   | 0.05 |
| 300     | 1.80    | 2.11  | -       | 0.06 |
| 400     | 4.63    | 4.92  | -       | 0.08 |
| 500     | 8.24    | 9.62  | -       | 0.11 |
| 600     | 15.92   | 16.51 | -       | 0.15 |
| 700     | 27.35   | 25.99 | -       | 0.20 |
| 800     | 42.57   | 39.37 | -       | 0.28 |

does not contain further optimisations. The computing time in Mathematica® (of the wrong result) sums up 4.32 seconds. It is worth recalling that the code of our programs in SML and Haskell has been generated from a verified algorithm.

Table 4 presents the times used to compute the inverse of matrices of elements in $\mathbb{R}$. Note that here both SML and Haskell are using double-precision floating-point numbers and thus numerical stability problems arise (the rref of matrices is not diagonal anymore, it contains small nonzero entries), as also happens in Sage. Once again, Poly/ML and MLton outperform Haskell. The comparison with Sage is better than in the previous cases.

Finally, in Table 5 we present the solution of systems of linear equations with coefficients in $\mathbb{Q}$ (with arbitrary precision). The times in Sage are divided into two different operations: the first one represents the time for obtaining a single solution, and the second one the time for computing a basis of the null space of the original matrix.

6 Conclusions and Further work

Formalisation of Mathematics is a rather challenging, and sometimes little rewarding, task. Formal proofs are considered deeply specific and remotely reusable, as well as very singular and concrete works. As an example, the Isabelle/HOL Library offers, to the best of our knowledge, three different repre-
sentations of matrices, each of them equally interesting and used for challenging works. Because of this, the field has received little attention along the years, even inside of the Formal Methods community (except for some groups of Computer Science theorists, usually the ones involved in the development of the tools). Nevertheless, the technology (both the hardware and the software) has improved along the last decades at such rate that nowadays it is possible to face challenges that were previously unthinkable.

Initiatives such as the Flyspeck project (lead by T. Hales, for the formalisation of the Kepler conjecture) and the classification of finite simple groups (by G. Gonthier) show that challenging results in Mathematics can be explored with proving assistants. They also pave the way for research in some other fields (for instance, algorithmics) where formalisation is also, at least, as relevant and required as in Mathematics (see the previous failures mentioned above, that could be critical in applications such as cryptology). In this field is where our work can be considered as a first milestone in the way to the formalisation of Linear Algebra algorithms; several of the tools that have been presented and already formalised in our work are reusable in Numerical Linear Algebra algorithms. For instance, some of the serialisations introduced in Section 4 are already part of the Isabelle Library. Several proofs of basic properties of elementary row and column operations are also reusable. Even with the simple version of the Gauss-Jordan algorithm presented and formalised in this work, the effort devoted and the results obtained pay off (formalisation of previously unconsidered results, real world applications in digital image processing, detection of commercial software bugs).

The amount of verified code generated in our work (ca. 2500 lines in each SML and Haskell) is considerable and covers a wide range of applications in Linear Algebra. Its formalisation (available in [5]) took 15000 lines of Isabelle code. The HMA Library infrastructure reduced significatively the amount of mathematical results to be formalised. A similar Library for Numerical Linear Algebra would help in future developments.

As a natural continuation to our work, our intention is now to provide a framework (and a methodology) in which the pieces presented here can be used to implement and formalise Numerical Linear Algebra algorithms in a more general way, and which does not require a deep Isabelle knowledge. The ideas (and

| Size (n) | Poly/ML | MLton | Sage |
|---------|---------|-------|------|
| 10      | 0.08    | 0.03  | 0.01 + 0.00 |
| 20      | 2.40    | 0.69  | 0.01 + 0.00 |
| 30      | 14.35   | 4.62  | 0.01 + 0.00 |
| 40      | 48.98   | 16.28 | 0.01 + 0.00 |
| 50      | 142.25  | 47.09 | 0.03 + 0.03 |
| 60      | 301.35  | 101.18| 0.02 + 0.03 |
| 70      | 603.56  | 202.46| 0.02 + 0.02 |
| 80      | -       | -     | 0.04 + 0.03 |
| 90      | -       | -     | 0.02 + 0.03 |
| 100     | -       | -     | 0.03 + 0.02 |

Table 5: Elapsed time (in seconds) to compute the solution of a system of linear equations with coefficients in $\mathbb{Q}$.
hopefully part of the technology) are borrowed from the Autoref tool [14] (also
developed in Isabelle/HOL), which facilitates the refinement of data types (as
we already did) and, more interestingly, algorithms over abstract concepts (sets,
maps) to algorithms over concrete implementations, and automatically gener-
ates the refinement theorems (that the user must prove). Consequently, one
must prove the properties of the original abstract algorithm (in which imper-
ative constructs are also permitted), and then ensure that the transformations
(perform by monadic refinements) preserve the original behaviour. Our origi-

data types would be vectors and matrices implemented as functions over
finite domains (this work shows that algorithmic formalisation is feasible within
these types), and algorithms over them, in a language closer to the one presented
in Algorithm 1 than to the Isabelle code snippets presented. Input algorithms
need not to be very optimised, to favour and simplify their formalisation. Addi-
tionally, the HMA Library offers a background to link the algorithms with their
original mathematical signification.

In this setting, refined algorithms over optimised data structures (such as
arrays) become the concrete implementation, whose formalisation shall emerge
from iterated refinements of the original (abstract) algorithm, paying attention
exclusively to the particular transformations performed (and not to the inherent
complexities of the optimised version). The idea has been successfully applied
with some intricate algorithms in automata theory [7]. We aim at applying it
to Numerical Linear Algebra specifications of algorithms and refining them to
compelling programs.

Incidentally, the methodology could also be applied to different fields of
Numerical Algebra where general simple algorithms are commonplace but special-
isged versions (or refinements) are widely used by the community.

A different research line would be to explore certifying algorithms. Certifying
algorithms permit to obviate the formalisation of the algorithm specification,
and focus on providing a certain output, and also a certificate (for instance,
in the form of a witness) that the output is correct with respect to some re-
quirements. Some of our computations are apparently amenable to this kind
of methodology (for instance, computing the solutions to a system of linear
equations and the fundamental subspaces). On the other hand, certifying the
computation of the rank, determinant and even the rref of a matrix could be, a
priori, as challenging as formalising them.

Acknowledgments

David Matthews, Matthew Fluet and Tjark Weber gave us valuable advice to
speed up our programs in SML and Poly/ML. David Matthews also modified
Poly/ML 5.5.1 to improve the performance offered by variable binders.

Juan Luis Varona helped us to perform Mathematica® computing tests and
gave us valuable information about this system. His work encourages formalisa-
tion efforts and consequently motivates ours.

This work has been supported by the research grant FPI-UR-12, from Uni-
versidad de La Rioja.
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