



Challenges of Symbolic Computation: My Favorite Open Problems[†]

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With an Additional Open Problem By

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*To Bobby F. Caviness
on the occasion of his 60th birthday*

The success of the symbolic mathematical computation discipline is striking. The theoretical advances have been continuous and significant: Gröbner bases, the Risch integration algorithm, integer lattice basis reduction, hypergeometric summation algorithms, etc. From the beginning in the early 1960s, it has been the tradition of our discipline to create software that makes our ideas readily available to scientists, engineers, and educators: SAC-1, Reduce, Macsyma, etc. The commercial viability of our system products is proven by Maple and Mathematica.

Today's user communities of symbolic computation systems are diverse: educators, engineers, stock market analysts, etc. The mathematics and computer science in the design and implementation of our algorithms are sophisticated. The research challenges in symbolic computation at the close of the twentieth century are formidable.

I state my favorite eight open problems in symbolic computation. They range from problems in symbolic/numeric computing, symbolic algorithm synthesis, to system component construction. I have worked on seven of my problems and borrowed one from George Collins. I present background to each of my problems and a clear-cut test that evaluates whether a proposed attack has solved one of my problems. An additional ninth open problem by Rob Corless and David Jeffrey on complex function semantics is given in an appendix.

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Introduction

At the *Fifth East Coast Computer Algebra Day*, which was held at the United States Naval Academy in Annapolis, Maryland, on April 25, 1998, I gave a 1 hour lecture of

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the same title. I repeated this lecture at the *IMACS Conference on Applications of Computer Algebra*, which was held in Prague, Czech Republic, on August 9–11, 1998. In this companion paper I have written up my favorite open problems of symbolic computation and provided a more in-depth discussion with references to the literature. The selection of open problems is my personal one and is not intended to be comprehensive of the field. I am leaving out major areas of investigation, among them differential and difference equations, types of domains in symbolic programming languages, computational group theory, or mathematics on the Internet. In an appendix to this paper, R. Corless and D. Jeffrey state an additional open problem, which was presented by Corless in his lecture at the same *Fifth East Coast Computer Algebra Day* in April 1998.

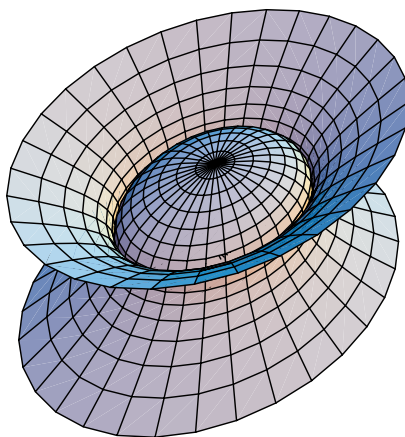
A BRIEF HISTORY OF SYMBOLIC MATHEMATICAL COMPUTATION

It is dangerous to stereotype historical development into periods. The following highlights during the decades of symbolic computation, as I perceive them, should simply be taken as a guideline.

- 1960s: pioneering years: polynomial arithmetic, integration
- 1970s: Macsyma and Reduce; abstract domains: Scratchpad/II
- 1980s: polynomial-time methods: factorization; Maple; user interfaces: Mathematica
- 1990s: teaching of calculus; math on the web; black box symbolic objects
- 2000s: merging of symbolic, numeric, geometric, combinatoric, and logic paradigm (?)

In the past 40 years or so the discipline of symbolic computation has made major contributions to science. Collins (1960) pioneered the process of automatic garbage collection by reference counts. New efficient multivariate polynomial greatest common divisor algorithms (see Brown, 1971, and the references given there) are crucial for the implementation of symbolic algebra. Risch (1969) showed that the problem of finding integrals of mathematical functions in closed form is decidable. Randomization was used by Berlekamp (1970) to efficiently factor polynomials modulo large prime numbers before the now well-known randomized primality tests. Generic programming was invented in the first half of the 1970s as a means to reuse the code of algebraic algorithms over abstract domains, such as Gaussian elimination (see Section 7). Gosper in 1978 invented an ingenious algorithm for indefinite hypergeometric summation (see Petkovšek *et al.*, 1996). Lovász's lattice reduction algorithm, a far-reaching generalization of the Euclidean algorithm, appeared first as a substep for polynomial factorization (Lenstra *et al.*, 1982). Interpolation algorithms for sparse multivariate polynomials, some of which are based on error-correcting coding, revise a numerical computation subject that is over 100 years old (see Grigoriev and Lakshman, 1995, and the references given there) and have become instrumental in the calculus of black box polynomials (Kaltofen and Trager, 1990). Today, the mathematical markup for Internet documents exposes several new issues, such as the structuring of compound objects for display and selection.[†] Last, but not least, we must mention the breakthrough algorithms for computing a Gröbner basis, which are discussed further in Section 5, and for solving a sparse linear system over abstract fields, which are discussed in more detail in Section 3.

[†]Oral communication by R. S. Sutor.



$$81x^4 + 16y^4 - 648z^4 + 72x^2y^2 - 648x^2 - 288y^2 + 1296 = (9x^2 + 4y^2 + 18\sqrt{2}z^2 - 36)(9x^2 + 4y^2 - 18\sqrt{2}z^2 - 36) = 0$$

Figure 1. Surface represented by a trivariate polynomial.

Our community of world-wide researchers is relatively small, between 150–300 active full-time researchers. I am sure, however, that we will continue to contribute in a significant way to science, and I hope that one or the other of the following nine problems will attract attention.

1. Symbolic/Numeric Computation

A surface that is defined implicitly by all real roots (x, y, z) of a trivariate polynomial is displayed in Figure 1. The picture indicates that there are two components, an ellipsoid and a hyperboloid, which the factorization of the polynomial over the complex numbers \mathbb{C} verifies.

Now we take the two factors, approximate $\sqrt{2}$ numerically by 1.41422 in one factor and 1.41421 in the other, and multiply the product out rounded to three decimal places. We obtain the numerical trivariate polynomial equation

$$81x^4 + 16y^4 - 648.001z^4 + 72x^2y^2 + 0.002x^2z^2 + 0.001y^2z^2 - 648x^2 - 288y^2 - 0.007z^2 + 1296 = 0.$$

Due to continuity the numerical perturbations do not change the picture of Figure 1 by much. The two now deformed components are still present. However, the polynomial has become absolutely irreducible over \mathbb{C} . My first open problem concerns the factorization of nearby polynomials over the complex numbers.

OPEN PROBLEM 1. Given is a polynomial $f(x, y) \in \mathbb{Q}[x, y]$ and $\epsilon \in \mathbb{Q}$. Decide in polynomial time in the degree and coefficient size if there is a factorizable $\hat{f}(x, y) \in \mathbb{C}[x, y]$ with $\|f - \hat{f}\| \leq \epsilon$, for a reasonable coefficient vector norm $\|\cdot\|$.

This problem was first posed in my survey article (Kaltofen, 1992). Efficient algorithms for performing the factorization of a multivariate polynomial over the complex numbers

exactly were described and cited in Kaltofen (1995). Galligo and Watt (1997) presented heuristics for computing complex numerical factors. Since then, I have learned of several related problems and their solution. They are described next. The constrained root problem described below solves Problem 1 if one looks for the nearest polynomial with a complex factor of degree no more than a given constant bound (Hitz *et al.*, 1999).

SENSITIVITY ANALYSIS: APPROXIMATE CONSISTENT LINEAR SYSTEM

Suppose the linear system $Ax = b$, where A is an $m \times n$ matrix over a field and b is a vector in an inner product space, is unsolvable. A classical problem is to find \hat{b} “nearest to” b that makes it solvable.

If nearness is measured in terms of the norm induced by the inner product, say if one wishes to minimize the Euclidean distance, $\min_{\hat{x}} \|A\hat{x} - b\|_2$, a solution is obtained by the method of least squares. Another important case is when the *component-wise* distance is minimized:

$$\min_{\hat{x}} \left(\max_{1 \leq i \leq m} \left| b_i - \sum_{j=1}^n a_{i,j} \hat{x}_j \right| \right).$$

By introducing a new variable y we can derive the minimum by solving the linear program due to Chebyshev.

$$\begin{aligned} &\text{minimize: } y \\ &\text{linear constraints: } \begin{aligned} y &\geq b_i - \sum_{j=1}^n a_{i,j} \hat{x}_j & (1 \leq i \leq m) \\ y &\geq -b_i + \sum_{j=1}^n a_{i,j} \hat{x}_j & (1 \leq i \leq m). \end{aligned} \end{aligned}$$

Component-wise minimization can account for round-off errors in the entries of b .

SENSITIVITY ANALYSIS: NEAREST SINGULAR MATRIX

There is no particular reason why one should not consider changes in A for finding solvable systems that are nearby. In fact, there exists a theory of so-called *total* least square methods (Golub and Van Loan, 1996). Related to it is the problem of finding the numeric rank of a non-singular matrix. Both problems are numerically attacked by computing the singular value decomposition of the matrix. Unfortunately, the results are not always satisfactory, and the following may explain why this is.

Consider the following mathematical question. Given are $2n^2$ rational numbers $\underline{a}_{i,j}, \bar{a}_{i,j}$. Let \mathcal{A} be the *interval* matrix

$$\mathcal{A} = \left\{ \left[\begin{array}{ccc} a_{1,1} & \cdots & a_{1,n} \\ \vdots & & \vdots \\ a_{n,1} & \cdots & a_{n,n} \end{array} \right] \mid \underline{a}_{i,j} \leq a_{i,j} \leq \bar{a}_{i,j} \text{ for all } 1 \leq i, j \leq n \right\}.$$

Does \mathcal{A} contain a singular matrix?

This problem has been shown to be *NP-complete* (Poljak and Rohn, 1993), i.e., it is computationally as difficult as computing the shortest traveling salesperson route in a complete graph. We mention Poljak’s and Rohn’s breakthrough reduction because it establishes that floating point roundoff errors may not always be easy to undo. When the distance is measured by a *matrix norm*, the problem of finding the nearest singular matrix can be solved efficiently by a result of Eckart and Young (1936) for Euclidean norms and of Gastinel (see Kahan, 1966) for arbitrary matrix norms.

corresponding differential equations (see Gantmacher, 1960, Chapter XV). There now exist many generalizations of Kharitonov’s theorem.

SENSITIVITY ANALYSIS: CONSTRAINED ROOT PROBLEM

Kharitonov’s theorem inspires new problem formulations in root stability. Given is a real or complex polynomial

$$f(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_1 z + a_0$$

and a root $\alpha \in \mathbb{C}$ that may be given explicitly or that may be constrained to a certain subset of \mathbb{C} . Compute \hat{f} “nearest to” f such that $\hat{f}(\alpha) = 0$.

We (Hitz and Kaltofen, 1998) can solve this problem efficiently, i.e., in polynomial time for the usual coefficient fields, and for:

- (1) a parametric α (root stability) and Euclidean distance,
- (2) explicit roots $\alpha_1, \alpha_2, \dots$ and coefficient-wise distance (infinity norm), and
- (3) with linear coefficient constraints, e.g. $a_n = 1$.

A theorem provable by our methods is the following (Hitz *et al.*, 1999). Given is the real polynomial

$$f(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0, \quad a_i \in \mathbb{R},$$

with no real root. Then one can compute in polynomial time in n and the size of the coefficients a_i the following quantity (Hitz *et al.*, 1999)

$$\min_{\substack{\hat{a}_0, \dots, \hat{a}_n \text{ such that} \\ \exists \alpha \in \mathbb{R}: \hat{a}_n \alpha^n + \hat{a}_{n-1} \alpha^{n-1} + \dots + \hat{a}_0 = 0}} \left(\max_{0 \leq i \leq n} |a_i - \hat{a}_i| \right) = \left| \frac{f(\alpha)}{\sum_{i=0}^n |\alpha^i|} \right|.$$

A related result appears in Zhi and Wu (1998).

2. Quantifier Elimination (QE)

What makes the approximation theoretic minimax problems of Section 1 decidable in the first place? The well-known process of quantifier elimination in the theory of real closed fields, first published by Tarski in 1948, delineates a substantial mathematical theory where all theorems are decidable and that has no Goedel-like undecidabilities. We illustrate the principle of QE on the simple example of minimizing a quadratic function.

$$\begin{aligned} \text{for } a > 0: \min_x (ax^2 + bx + c) &\iff \forall y: a > 0 \text{ and } ay^2 + by + c \geq ax^2 + bx + c \\ &\iff a > 0 \text{ and } x = -\frac{b}{2a}. \end{aligned}$$

The minimizing problem can be rewritten as a quantified expression. The principle of QE allows the removal of the quantified variables—our equivalent third form. All values of the variables that satisfy any quantifier-free expression define a so-called *semi-algebraic* set. By QE those specializations of the free variables of a quantified expression that yield theorems, i.e., true formulas, form a semi-algebraic set. The algorithmic aspects of QE have been studied extensively by G. Collins, D. Grigoriev, J. Renegar, H. Hong, and others (see Caviness and Johnson, 1998). In general, the process is computationally

hard, although several of the examples in Section 1 have efficient algorithms. Collins has suggested another minimax problem as a challenge benchmark problem for QE software with the intent to demonstrate the abilities of the different algorithms and their implementations.

OPEN PROBLEM 2. (ZOLOTAREV’S PROBLEM BY COLLINS, 1992) Eliminate the quantifiers and solve for $n \geq 6$ on a computer:

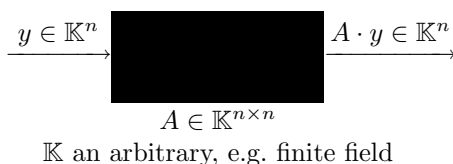
$$\text{for } r > 0: \min_{B=b_0+\dots+b_{n-2}x^{n-2}} \left(\max_{-1 \leq x \leq 1} |x^n + rx^{n-1} - B(x)| \right).$$

The best approximation of a polynomial of degree n by a polynomial of lower degree on the interval $\{x \mid -1 \leq x \leq 1\}$ is accomplished via Chebyshev polynomials. Zolotarev sought best approximations by polynomials whose degree is at least 2 less. Note that mathematical expressions for explicit solutions are known (see Achiezer, 1956, Addendum E) and we give the one for $r \leq 1$ and $n = 3$, again in the form of a formula in Tarski’s theory.

$$\forall c_0, c_1 \forall x \exists y: (0 < r \leq 1 \text{ and } -1 \leq x \leq 1 \text{ and } -1 \leq y \leq 1) \Rightarrow (y^3 + ry^2 - c_1y - c_0)^2 \geq \left(x^3 + rx^2 - \underbrace{\left(\frac{3}{4} + \frac{r}{2} - \frac{r^2}{4} \right)}_{b_1} x - \underbrace{\left(\frac{r}{4} + \frac{r^2}{6} - \frac{r^3}{108} \right)}_{b_0} \right)^2.$$

3. Linear Algebra With Implicitly Represented Matrices

Several numerical methods for solving systems of linear equations with sparse coefficient matrices are based on the use of not too many matrix-times-vector products, which in the sparse case can be performed quickly. Examples for such methods are the conjugate gradient, the Lanczos and the Krylov algorithms. These methods are sometimes referred to as matrix-free, because no coefficient matrix needs to be explicitly constructed. In 1990 we introduced the notions of black box polynomials, rational functions, and matrices (Kaltofen and Trager, 1990). The black box model of a matrix requires as the representation of a matrix a function that performs the matrix-times-vector product.



In the symbolic computation context we consider abstract coefficient fields, such as finite fields. The main objective is to perform all linear algebra operations, e.g. $A^{-1}b$ (Wiedemann, 1986) with

$$\begin{array}{ll} O(n) & \text{black box calls and} \\ n^2(\log n)^{O(1)} & \text{arithmetic operations in } \mathbb{K} \text{ and} \\ O(n) & \text{intermediate storage for field elements.} \end{array} \tag{3.1}$$

Table 1. Flurry of recent results.

Lambert (1996), Teitelbaum (1998), Eberly and Kaltofen (1997)	relationship of the Wiedemann and Lanczos approach
Villard (1997a,b)	analysis of the <i>block</i> Wiedemann algorithm
Giesbrecht (1997), Mulders and Storjohann (1999)	computation of integral solutions
Giesbrecht <i>et al.</i> (1998)	certificates for inconsistency

We note that a black box matrix algorithm applies not only to sparse matrices but also to structured matrices that have a fast matrix-times-vector function. Fast matrix-times-vector products are often a consequence of the linearization of a given problem. Examples are:

- (1) Petr's Q matrix in Berlekamp's algorithm for factoring polynomials over finite fields (Knuth, 1997; Kaltofen and Shoup, 1998).
- (2) resultant matrices for non-linear algebraic equations (see Section 5 below).
- (3) the linear systems in Kaltofen's (1995) algorithm for factoring multivariate polynomials over algebraically closed fields.

Linear algebra algorithms for black box matrices are an active subject of research. In Table 1 we list several of them. Giesbrecht's (1997) method for finding integral solutions to sparse linear systems is based on computing rational solutions whose denominators are relatively prime. For instance, if one obtains two rational solutions with common denominator 2 and 3, respectively, one can easily construct an integer solution.

$$A\left(\frac{1}{2}x^{[1]}\right) = b, x^{[1]} \in \mathbb{Z}^n, \quad A\left(\frac{1}{3}x^{[2]}\right) = b, x^{[2]} \in \mathbb{Z}^n;$$

$$\gcd(2, 3) = 1 = 2 \cdot 2 - 1 \cdot 3, \quad A(2x^{[1]} - x^{[2]}) = 4b - 3b = b.$$

Giesbrecht proceeds by proving that for a small algebraic extension of \mathbb{Z} relative primeness occurs with high probability. Recently, the need for small algebraic extension has been removed (Mulders and Storjohann, 1999).

Since Wiedemann's (1986) breakthrough paper, the following problem remains unresolved.

OPEN PROBLEM 3. Within the resource limitations (3.1) stated above,[†] compute the characteristic polynomial of a black box matrix over an abstract field. Randomization is allowed (of course!), as is a "Monte Carlo" solution.

Characteristic polynomials are needed, for example, for resultant computations (Canny *et al.*, 1989; Canny, 1990; Emiris and Pan, 1997). We conclude this section by remarks on Monte Carlo vs. Las Vegas randomized algorithms.

[†]Joachim von zur Gathen has suggested relaxing the $O(n)$ requirements for both the number of black box calls and for intermediate auxiliary storage to $n(\log n)^{O(1)}$.

CLASSES OF RANDOMIZED ALGORITHMS

The use of random bits, so-called coin flips, has turned out to be a powerful algorithm design tool. Coin flips are employed for both speed, i.e., for locating the solution by a random walk rather than by deterministic search, and for output correctness, where unverifiable guesses about the solution are made. The latter comes from numerical integration: the frequency, with which a random point in space is below a function, is used to approximate the integral of the function. The following notions have become popular:

Monte Carlo	≡	always fast, probably correct
Las Vegas	≡	always correct, probably fast
BPP	≡	probably correct, probably fast

Here BPP stands for bounded probabilistic polynomial time and is a notion from complexity theory (Boppana and Hirschfeld, 1989). The complexity class R contains all problems solvable in Las Vegas polynomial time. The term Las Vegas was coined by Babai (1979). Clearly, as Gene Cooperman has pointed out to me, a BPP method can be converted to a Monte Carlo method by returning garbage when the random walk consumes too much time. It is unknown if $BPP = R$, or if $R = P$, the class of problems solvable deterministically in polynomial time. Many theorists conjecture that since randomized algorithms perform very well when implemented with pseudo-random number generators (Knuth, 1997, Chapter 3), coin flips are inessential for polynomial-time algorithmic solutions of problems. The practicality of such de-randomization is even further remote.

Some of my colleagues have expressed to me that Las Vegas randomization is fine, but Monte Carlo or BPP algorithms are suspicious as one cannot verify the guessed solution. I believe that such arguments are questionable. A Monte Carlo algorithm can deliver an answer that is correct with a probability that is as high as the user demands, e.g. higher than $1 - 1/2^{100}$. Of course, the probability of correctness can only be guaranteed if one uses a truly random process for the coin flips, say a quantum-physical effect. However, deterministic algorithms can also fail due to momentary hardware faults and programming bugs. Would the reader really trust a long number-theoretic proof together with a 10 000 line program more than the answer given by a single-page Monte Carlo primality testing program (Knuth, 1997, Section 4.5.4)?

We have observed a further pitfall when trying to use Las Vegas algorithms. The following scheme is often employed, which makes a Monte Carlo algorithm Las Vegas by verifying its answer by alternative considerations.

```

repeat
    pick random numbers
    compute candidate answer
until a solution passes a test for it

```

The scheme has the flaw that a programming bug leads to an infinite loop, which is indistinguishable from bad luck in the coin flips! I have been told by many of my colleagues that such looping has also happened to them. Eventually, we give up in the

belief that the coin flips keep on being unlucky and begin searching for the bug. In one case, the problem turned out to be an invalid input.

A referee points out that even sequential schemes with unbounded iteration have this flaw. For instance, in Brown's (1971) modular GCD algorithm, the Chinese remaindering is stopped if the division check by the GCD candidate succeeds. Due to our experience (Kaltofen and Monagan, 1999) we now advocate avoiding such unbounded loops whenever possible, even when adding a small extra cost.[†]

4. Lattice Basis Reduction

The lattice basis reduction algorithm by Lenstra *et al.* (1982) is said to be the major algorithmic breakthrough of symbolic computation in the 1980s (Odlyzko, 1996). The first application of the method was to factoring polynomials over the rational numbers. Since 1982 the algorithm had its impact on a variety of problems (see, e.g. Borwein and Lisoněk, 1997). Recently, the method was used to derive the following pretty formula for π .

$$\pi = \sum_{i=0}^{\infty} \frac{1}{16^i} \left(\frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6} \right). \quad (4.2)$$

Following Bailey *et al.* (1997), one proceeds as follows. Each term under the sum (4.2) can be expressed as an integral multiple of a rational integral.

$$\int_0^1 \frac{y^{k-1}}{1 - \frac{y^8}{16}} dy = \int_0^1 \sum_{i=0}^{\infty} y^{k-1} \left(\frac{y^8}{16} \right)^i dy = \sum_{i=0}^{\infty} \frac{1}{16^i} \int_0^1 y^{8i+k-1} dy = \sum_{i=0}^{\infty} \frac{1}{16^i(8i+k)}.$$

The question is which integer linear combination of these integrals yields π . Lattice basis reduction is used to find the multipliers. First, we approximate π and the integrals, multiplied by 10^{25} , via a Maple V procedure. Note that the global variable `Digits` in Maple holds the number of decimal mantissa digits with which Maple performs its floating point arithmetic.

```
> latt := proc(digits)
> local k, j, v, saved_Digits, ltt;
> saved_Digits := Digits; Digits := digits;
> for k from 1 to 8 do
>   v[k] := [];
>   for j from 1 to 10 do v[k] := [op(v[k]), 0]; od;
>   v[k][k] := 1;
>   v[k][10] := trunc(10^digits *
>                     evalf(Int(y^(k-1)/(1-y^8/16),
>                               y=0..1, digits), digits));
> od;
> v[9] := [0,0,0,0,0,0,0,0,1,
>          trunc(evalf(Pi*10^digits,digits+1))];
> ltt := [];
> for k from 1 to 9 do ltt:= [op(ltt),evalm(v[k])]; od;
```

[†]A similar programming philosophy has also been expressed by Kurt Mehlhorn for building the LEDA library.

```

> Digits := saved_Digits;
> RETURN(ltt);
> end:
> L := latt(25);

```

```

L := [[1, 0, 0, 0, 0, 0, 0, 0, 0, 10071844764146762286447600],
      [0, 1, 0, 0, 0, 0, 0, 0, 0, 5064768766674304809559394],
      [0, 0, 1, 0, 0, 0, 0, 0, 0, 3392302452451990725155853],
      [0, 0, 0, 1, 0, 0, 0, 0, 0, 2554128118829953416027570],
      [0, 0, 0, 0, 1, 0, 0, 0, 0, 2050025576364235339441503],
      [0, 0, 0, 0, 0, 1, 0, 0, 0, 1713170706664974589667328],
      [0, 0, 0, 0, 0, 0, 1, 0, 0, 1472019346726350271955981],
      [0, 0, 0, 0, 0, 0, 0, 1, 0, 1290770422751423433458478],
      [0, 0, 0, 0, 0, 0, 0, 0, 1, 31415926535897932384626434]].

```

If π is an integer linear combination of the integrals, the above lattice vectors must sum to a short vector, which can be determined by lattice basis reduction (Håstad *et al.*, 1989) or the PSLQ algorithm (Ferguson and Bailey, 1996).

```

> readlib(lattice):
> lattice(L);

```

```

[[-4, 0, 0, 2, 1, 1, 0, 0, 1, 5], [0, -8, -4, -4, 0, 0, 1, 0, 2, 5],
 [-61, 582, 697, -1253, 453, -1003, -347, -396, 10, 559],
 [-333, 966, 324, -1656, -56, 784, 1131, -351, -27, 255],
 [429, 714, -1591, 778, -517, -1215, 598, 362, -87, 398],
 [-1046, -259, -295, -260, 1286, 393, 851, 800, 252, -1120],
 [494, 906, -380, -1389, 1120, 1845, -1454, -926, -218, 400],
 [1001, -1099, 422, 1766, 1405, -376, 905, -1277, -394, -30],
 [-1144, 491, -637, -736, -1261, -680, -1062, -1257, 637, -360]].

```

The first short vector corresponds to (4.2). The second vector is another linearly independent solution:

$$2\pi = \sum_{i=0}^{\infty} \frac{1}{16^i} \left(\frac{8}{8i+2} + \frac{4}{8i+3} + \frac{4}{8i+4} - \frac{1}{8i+7} \right). \quad (4.3)$$

One may use Maple V.4 directly to complete the proof of (4.3) by carrying out the corresponding integral symbolically.

```

> g := (8*y + 4*y^2 + 4*y^3 - y^6)/(1-y^8/16);

```

$$g := \frac{8y + 4y^2 + 4y^3 - y^6}{1 - \frac{1}{16}y^8}$$

```

> int(g, y=0..1);

```

2 π .

Formulas like (4.2) and (4.3) can be used to compute the binary digits of π at very high position without keeping track of the intermediate expansion, the so-called spigot algorithm. At this moment, no formula that allows the computation of decimal digits in this space and time efficient manner is known.

THE GGH PUBLIC KEY CRYPTOSYSTEM

Recently, the properties of reduced lattice bases have been employed to design public key cryptosystems. Here is a nutshell description of the one by Goldreich *et al.* (1997b).

Public key A lattice basis B (rows B_i are basis vectors).

Private key A *reduced* basis C for lattice spanned by the rows of B .

Clear text Represent the message as a vector x with *small* integer entries.

Encoded message $y = x + \sum_i r_i B_i$ where $\sum_i r_i B_i$ is a random vector in the lattice.

Decryption is based on one of Babai's (1986) algorithms for nearest lattice point: write $y = \sum_i s_i C_i$ with $s_i \in \mathbb{Q}$. Then $\sum_i \text{nearest-integer}(s_i) C_i$ is a near lattice point, probably $\sum_i r_i B_i$.

In the paper by Goldreich *et al.* (1997b), more details are given on how to choose B and C and how to sample random lattice points so that the decryption method does not produce an incorrect near lattice point. Nonetheless, Phong Nguyen has been able to break this scheme in about 3 days on a 140 MHz Ultrasparc using NTL 1.7's Schnorr-Euchner variant of the reduction algorithm for lattices of dimension 200. An alternative cryptosystem is described in Ajtai and Dwork (1997) and Goldreich *et al.* (1997a) and proven secure provided that computing a short non-zero lattice vector is hard.

OPEN PROBLEM 4. Devise a public key cryptosystem that is based on diophantine linear algebra but that is safe from lattice basis reduction.

5. Gröbner Bases

The classical tool for solving a system of non-linear algebraic equations is the u-resultant. Consider the following simple example, due to Lazard (1981).

$$\begin{aligned} f_1 &= x^2 + xy + 2x & + & y - 1 = 0 & (x, y) &= (1, -1), (-3, 1), (0, 1) \\ f_2 &= x^2 & + & 3x - y^2 + 2y - 1 = 0 \\ f_3 &= & ux & + vy + w. \end{aligned}$$

By the theory of Macaulay (1916), the u-resultant can be expressed as the determinant of a matrix whose rows represent the polynomials multiplied by certain terms and whose

columns are labeled by certain terms whose coefficients are the entries.

$$\begin{array}{l}
 xf_1 \\
 yf_1 \\
 f_1 \\
 xf_2 \\
 yf_2 \\
 f_2 \\
 xyf_3 \\
 xf_3 \\
 yf_3 \\
 f_3
 \end{array}
 \begin{array}{c}
 \left| \begin{array}{cccccccccc}
 x^3 & x^2y & x^2 & xy^2 & xy & x & y^3 & y^2 & y & 1 \\
 1 & 1 & 2 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\
 0 & 1 & 0 & 1 & 2 & 0 & 0 & 1 & -1 & 0 \\
 0 & 0 & 1 & 0 & 1 & 2 & 0 & 0 & 1 & -1 \\
 1 & 0 & 3 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\
 0 & 1 & 0 & 0 & 3 & 0 & -1 & 2 & -1 & 0 \\
 0 & 0 & 1 & 0 & 0 & 3 & 0 & -1 & 2 & -1 \\
 0 & u & 0 & v & w & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & u & 0 & v & w & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & u & 0 & 0 & v & w & 0 \\
 0 & 0 & 0 & 0 & 0 & u & 0 & 0 & v & w
 \end{array} \right.
 \end{array}
 =
 \begin{array}{l}
 (u-v+w) \\
 \cdot (-3u+v+w) \\
 \cdot (v+w) \\
 \cdot (u-v) \\
 \\
 \text{(u-resultant)}
 \end{array}$$

The u-resultant has linear factors provided the system has a finite solution. Its coefficients are the coordinates of the zeros of the system, including solutions at infinity.

BUCHBERGER'S ALGORITHM

The concept of a Gröbner basis (Buchberger, 1965, 1970, 1985; Becker and Weispfenning, 1993; Cox *et al.*, 1996) has revolutionized commutative algebra. Buchberger's algorithm provides an alternative for solving non-linear algebraic systems. Within the algorithm, some S-polynomial constructions and reductions can be interpreted as row reduction in Macaulay's matrices, like the one given for the u-resultant above. Faugère (1998) has been able to make this correspondence more precise. In particular, his method uses sparse so-called symbolic LU matrix decomposition for efficiently performing these row reductions. His implementation may be the first major marriage of symbolic and numeric methods. The symbolic sparse LU factorization is purely combinatorial and treats the coefficient arithmetic abstractly. In Faugère's implementation the rational coefficients still become exceedingly large, and some computations can only be done modulo a prime number. Many other numeric sparse solvers benefit from iterative approximation of the solution, and my next problem suggests doing the same for Gröbner basis computation.

OPEN PROBLEM 5. Compute Gröbner bases approximately by iterative methods for solving systems, such as Gauss-Seidel, conjugate gradient, Newton, . . . A solution plugs into numerical software and computes some bases faster than by exact arithmetic; the structure of the bases may be determined, e.g. by modular arithmetic.

We note that related aspects of numerical error analysis are discussed in Shirayanagi (1996) and Stetter (1996).

6. Transposed Matrix Products

The following phenomenon has been observed in a variety of settings. One has an efficient algorithm for computing a linear map, but one actually needs the transposed map. We shall begin with an example from field theory.

We first describe the overall approach. Let $\sigma \in \mathbb{K}(\alpha, \beta)$ where

$$\begin{array}{ll}
 g = y^2 - 2 \in \mathbb{K}[y], & f = x^2 - y - 1 \in \mathbb{K}[x, y], \\
 \beta = (y \bmod g) \in \mathbb{K}[y]/(g), & \alpha = (x \bmod (f, g)) \in \mathbb{K}[x, y]/(f, g),
 \end{array}$$

with $\mathbb{K}[y]/(g) \subset \mathbb{K}[x, y]/(f, g)$. Note that $f(\alpha, \beta) = 0$ and $g(\beta) = 0$. For example, $\sigma = \sqrt{1 + \sqrt{2}} - \sqrt{2} = \alpha - \beta$. In field theoretic terms, σ is an algebraic element in a tower of fields $\mathbb{K} \subset \mathbb{K}(\beta) \subset \mathbb{K}(\alpha, \beta)$. The tower is represented by a triangular set of minimum polynomials for the extension elements α and β : $g \in \mathbb{K}[y]$ irreducible over \mathbb{K} , $f \in \mathbb{K}(\beta)[x]$ irreducible over $\mathbb{K}(\beta)$.

The computational task is to compute the minimum polynomial $h(\sigma) = 0$:

$$h(x) = x^m - c_{m-1}x^{m-1} - \dots - c_0 \in \mathbb{K}[x], \quad m \leq \deg(f) \cdot \deg(g).$$

The coefficient vectors $\vec{\sigma}^i$ of $\sigma^i \bmod (f(x, y), g(y))$ satisfy the linear recurrence on vectors

$$\forall j \geq 0: \vec{\sigma}^{m+j} = c_{m-1}\vec{\sigma}^{m-1+j} + \dots + c_0\vec{\sigma}^j.$$

Any non-trivial linear projection map $\mathcal{L}(\vec{\sigma}^i)$ preserves the linear recursion because h is irreducible. An algorithm can proceed by computing the field elements $a_i = \mathcal{L}(\vec{\sigma}^i)$ for $0 \leq i \leq 2m - 1$, i.e., using a linear map into \mathbb{K} , and from them the linear recurrence h , the latter in $m^{1+o(1)}$ field operations in \mathbb{K} by the Berlekamp/Massey algorithm (Massey, 1969; Brent *et al.*, 1980). We now inspect the task of computing the linear projections of the powers of σ in more detail.

POWER PROJECTIONS = TRANSPOSED MODULAR POLYNOMIAL COMPOSITION

The operator \mathcal{L} is represented by a vector of field elements $[u_0 \ u_1 \ \dots \ u_{n-1}]$, where $n = \deg(f) \deg(g)$. The power projections can be expressed by the following vector-times-matrix product:

$$\left[\mathcal{L}(\vec{\sigma}^0) \ \mathcal{L}(\vec{\sigma}^1) \ \mathcal{L}(\vec{\sigma}^2) \ \dots \right] = [u_0 \ u_1 \ \dots \ u_{n-1}] \cdot \underbrace{\left[\begin{array}{c|c|c|c} \vec{\sigma}^0 & \vec{\sigma}^1 & \vec{\sigma}^2 & \dots \end{array} \right]}_A.$$

The key observation is that the transposed linear map is modular polynomial composition:

$$w(z) = w_0 + w_1z + w_2z^2 + \dots \mapsto w(\sigma) \bmod (f(x, y), g(y))$$

$$\vec{w}(\sigma) = \underbrace{\left[\begin{array}{c|c|c|c} \vec{\sigma}^0 & \vec{\sigma}^1 & \vec{\sigma}^2 & \dots \end{array} \right]}_A \cdot \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \end{bmatrix}.$$

We note that modular polynomial composition in the univariate case has been studied extensively, as its complexity is closely related to factoring univariate polynomials over finite fields efficiently (von zur Gathen and Shoup, 1992; Kaltofen and Shoup, 1997, 1998; Bernstein, 1998; von zur Gathen and Gerhard, 1999).

The use of power projections for finding minimum polynomials of algebraic numbers and its relation to modular polynomial composition is discussed in Shoup (1994, Section 3). The special cases

$$\sigma = \alpha \pm \beta, \sigma = \alpha \cdot \beta, \sigma = \alpha/\beta \quad \text{with } f, g \in \mathbb{K}[x],$$

i.e., arithmetic operations on roots of polynomials, can be handled alternatively by resultant computations (Loos, 1982). These require the factorization of a polynomial of degree

$\deg(f) \cdot \deg(g)$ over \mathbb{K} , while our approach requires the factorization of f over $\mathbb{K}(\beta)$ or of g over $\mathbb{K}(\alpha)$, which is performed similarly by either a factorization of a resultant over \mathbb{K} (Trager, 1976; Encarnación, 1997), or by completely different and in some cases more efficient algorithms (Weinberger and Rothschild, 1976; Lenstra, 1987).

Nonetheless, we still have to compute the power projections. An algorithmic theorem, which we call *transposition principle*, now states that any linear algorithm that computes a matrix-times-vector product can be transformed into one that computes the transposed matrix-times-vector product. One simply reverses the flow of the linear circuit that represents the algorithm.[†] Such reversal of flow preserves the number of arithmetic operations, but not the space needed to store intermediate results. Therefore, a fast modular polynomial composition algorithm yields one for power projections, at least in theory. Shoup (1995) proceeded differently and designed, for the case of a single algebraic extension, a baby step/giant step algorithm based on modular polynomial multiplication. Again, he needed the transposed map for which he synthesized the following algorithm (see Shoup, 1995, for more details).

TRANSPosed MODULAR POLYNOMIAL MULTIPLICATION IN NTL

- (1) $T_1 \leftarrow \text{FFT}^{-1}(\text{RED}_k(g))$
- (2) $T_2 \leftarrow T_1 \cdot S_2$
- (3) $v \leftarrow -\text{CRT}_{0\dots n-2}(\text{FFT}(T_2))$
- (4) $T_2 \leftarrow \text{FFT}^{-1}(\text{RED}_{k+1}(x^{n-1} \cdot v))$
- (5) $T_2 \leftarrow T_2 \cdot S_3$
- (6) $T_1 \leftarrow T_1 \cdot S_4$
- (7) Replace T_1 by the 2^{k+1} -point residue table whose j th column ($0 \leq j < 2^{k+1}$) is 0 if j is odd, and is column number $j/2$ of T_1 if j is even.
- (8) $T_2 \leftarrow T_2 + T_1$
- (9) $u \leftarrow \text{CRT}_{0\dots n-1}(\text{FFT}(T_2))$

The algorithm has no interpretation of its own.[‡]

“we offer no other proof of correctness other than the validity of this transformation technique (and the fact that it does indeed work in practice)” (Shoup, 1995, Section 7.5)

It is, however, as time and space efficient as modular polynomial multiplication, and one is left with the question of whether the transposition principle has this property in general. Here then is our sixth open problem.

OPEN PROBLEM 6. With inputs $A \in \mathbb{K}^{m \times n}$ and $y \in \mathbb{K}^n$ you are given an algorithm for $A \cdot y$ that uses $T(m, n)$ arithmetic field operations and $S(m, n)$ auxiliary space. Show how to construct an algorithm for $A^T \cdot z$, where $z \in \mathbb{K}^m$, that uses $O(T(m, n))$ time and simultaneously $O(S(m, n))$ space. Your construction must be applicable to practical problems.

[†]The history of the principle is manifold. Bürgisser *et al.* (1997) traced it to circuit analysis (see Antoniou, 1979, Section 4.7). Fiduccia derived the principle in his Ph.D. Thesis (1973) (see also Fiduccia, 1972) and Kaminski *et al.* (1988) published a paper on it.

[‡]In the meantime, Shoup (1999) has been able to derive an explicit fast algorithm for the transposed modular polynomial multiplication problem. However, his algorithm is still by a constant factor slower than the one based on the transposition principle.

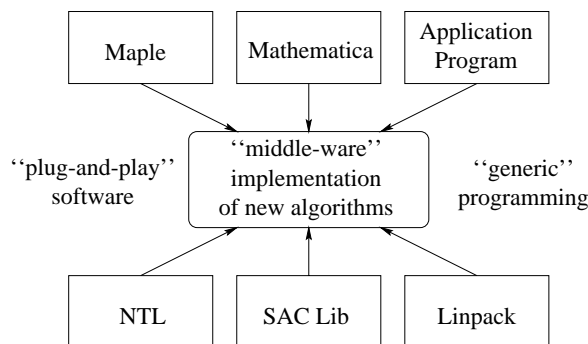


Figure 2. Component interaction in symbolic computation.

The transposition principle is a special case of *automatic differentiation* (Kaltofen and Lakshman, 1988):

$$\text{For } f(x_1, \dots, x_n) = b^T \begin{pmatrix} A \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \end{pmatrix} \text{ we have } \begin{bmatrix} \partial_{x_1} f \\ \vdots \\ \partial_{x_n} f \end{bmatrix} = A^T b.$$

Therefore, the so-called *reverse mode* of automatic differentiation for computing the gradient vector of a function applies. Griewank (1992) shows how to solve the above problem with a factor of $O(\log(mn))$ penalty in both time and space.

We conclude by noting that the Lanczos algorithms and certificates of inconsistency of Table 1 all depend on efficient transposed matrix-times-vector products.

7. Plug-And-Play Components

The notion of plug-and-play components comes from the interaction between computer hardware and the resident operating system. If new hardware is installed, the operating system can probe the device and determine and configure its characteristics without human help. The device must respond to the probes in an agreed fashion and the operating system must know of the possible different device characteristics. The question arises of whether a plug-and-play approach can be realized for the purpose of arranging software components in a customized fashion.

An example for the need of the plug-and-play methodology is given in Figure 2. A new algorithm, say the solution to Problem 1, is to be made available to researchers outside the discipline of symbolic computation. We assume that the users work on commercial platforms such as Maple, Mathematica, or an Internet browser/Java engine. Clearly, it is desirable to implement the brand-new algorithm in such a way that it is callable from these common platforms. Loos (1974) recognized the need as vertical integration.

A second issue concerns the usage of existing libraries, say for polynomial arithmetic or arbitrary precision floating point arithmetic. Computer algebra has pioneered what is now called *generic programming*, where the underlying implementations are hidden and multiple packages can be used, even at the same time. Generic programming was introduced simply because it became unwieldy to write a Gaussian elimination procedure, for example, for each of the different coefficient fields that arose. Now generic programming

has become a means of technology transfer. When a new sparse symbolic LU factorization algorithm is released in Linpack, that algorithm should be instantaneously called from all programs that rely on sparse LU factorization.

The notion of *problem-solving environments* has been coined. We offer plug-and-play and generic programming software design as a definition. With it an end-user can easily custom-make symbolic software tools.

EXAMPLE: FOXBOX (DÍAZ AND KALTOFEN, 1998)

One goal of our implementation of the algorithms for factoring polynomials in so-called black box representation (Kaltofen and Trager, 1990) was a plug-and-play interface to our FOXBOX system. Our Maple server makes the procedures in FOXBOX accessible to a Maple session. These are a Maple user's commands.

```
# Call FoxBox server from Maple
> SymToeQ := BlackBoxSymToe( BBNET_Q, 4, -1, 1.0 ):
> SymToeZP := BlackBoxSymToe( BBNET_ZP, 4, -1, 1.0 ):
> FactorsQ := BlackBoxFactors( BBNET_Q, SymToeQ, Mod, 1.0, Seed ):
> FactorsZP := BlackBoxHomomorphicMap( BBNET_FACS, FactorsQ, SymToeZP ):
```

The server program is a generic one. Here we give a code fragment of the version that uses SACLIB 1.1 rational number and polynomial arithmetic. The C++ constructor calls get compiled from the FOXBOX template library.

```
// construct factors of a symmetric Toeplitz determinant in C++
typedef BlackBoxSymToeDet< SaclibQ, SaclibQX > BBSymToeDetQ;
typedef BlackBoxFactors< SaclibQ, SaclibQX, BBSymToeDetQ > BBFactorsQ;

BBSymToeDetQ SymToeDetQ( N );
BBFactorsQ FactorsQ( SymToeDetQ, Probab, Seed, &MPCard );
```

SOFTWARE DESIGN ISSUES

We think it is useful to distinguish the plug-and-play interface from the generic programming interface, although the two are somewhat similar. We have identified several issues with both methodologies.

PLUG-AND-PLAY

- (1) The software components create a standard *serialized representation* for exchanging their data. For mathematical objects several standards have been proposed: MP (Bachman *et al.*, 1997), OpenMath (Dalmas *et al.*, 1997), and MathML (Ion and Miner, 1998). All standards use static representation of the objects.
- (2) In FOXBOX we could from the beginning transfer procedures for making or evaluating polynomials and matrices. Our procedures were written in standard programming languages, e.g. in C++, as security from illegal operations was not an issue.

Following the Java paradigm, it will be useful to transfer *byte code* for constructing objects in place of the parse trees for their canonical representation (cf. Norman and Fitch, 1996). The matrix $[1/(i^2 + j^2)]_{1 \leq i, j \leq 100}$ surely should be communicated via a procedure for constructing it. A standard for the mathematical byte code solves the task.[†]

- (3) Problem-solving environments (PSEs) (Lakshman *et al.*, 1998) are the end product of the assembly of the different software components. *Visual-programming environments* for instantiation of generic and assembly of plug-and-play components can become part of the user interface to symbolic computation systems, and assist the end-user in making her/his PSE, who thus unwittingly turns into a very high-level programmer.
- (4) A language that allows *overloaded operators* permits the wrapping of existing code with new definitions for the operators. MITMatlab (Husbands *et al.*, 1998) is an example where parallelism is introduced in this manner without having to modify sequential library functions.

GENERIC PROGRAMMING

- (1) The definition of *common object interfaces* has been studied extensively in the context of computer algebra (Musser, 1975; Abdali *et al.*, 1986; Jenks and Sutor, 1992; Monagan, 1993; Watt *et al.*, 1994). The Standard Template Library of C++ (Musser and Saini, 1996) is an example from main-stream programming. STL has container objects with a standardized format for manipulating them.[‡] Such standards can be created for mathematical objects such as polynomials, matrices, or combinatorial graphs. Libraries are then accessed through so-called wrapper classes that convert the standard calling interface to the internal organization. No efficiency is lost, as the wrapper functions can be inlined on compilation. In FOXBOX the wrapper classes provide streams of objects. For instance, `K::random_generator(500)` is a generic function object of the field class that provides random field elements that are uniformly sampled from a set of 500 elements. Random field elements are needed for randomized algebraic algorithms (cf. Section 3). Specification of the object interfaces can be expressed in CORBA, the Common Object Request Broker Architecture (Iglío and Attardi, 1998).
- (2) Several libraries, e.g. SACLIB, perform *garbage collection*, which complicates the generic object interface. Explicit *storage management* remains a sticky issue even in STL, as different C++ compilers implement different memory models.
- (3) *Exceptions*, such as division by zero or failure due to an unlucky selection of random elements, must be handled in a generic fashion across the components.
- (4) Object interfaces sometimes become a barrier that disallows interaction between the generic algorithm and the used generic arithmetic. For instance, a ring of polynomials whose arithmetic is implemented by FFT-based methods, such as in NTL (Shoup, 1998), has an efficient specialized evaluation/interpolation scheme. The generic algorithms can use a *shortcut* into the specialized procedures when employing a homomorphic imaging strategy. The wrapper classes can facilitate these shortcuts.

[†]The OpenMath “programming content dictionary” proposed by Gaston Gonnet offers a possible solution.

[‡]STL does not supply a standard for serializing its containers for transport across systems.

Table 2. Successful applications.

Product	“Killer application”
Macintosh	Document preparation
Personal computer	Spreadsheets
Supercomputers	Weather forecasting
Mainframe computers	Social security system
Symbolic software	Calculus teaching

- (5) *Parallel distribution* of a symbolic computation over many different computers is important as our computations tend to be large. Internet browsers can present a familiar platform for managing the network of computers one utilizes. The algorithms must be programmed with high-level parallelization that is built-in from the beginning.

OPEN PROBLEM 7. Devise a plug-and-play and generic programming methodology for symbolic mathematical computation that is widely adopted by the experts in algorithm design, the commercial symbolic software producers, and the outsider users.

From our FOXBOX experience I observed that designing a system that simultaneously plugs into several others is difficult. H. Hong, a co-author of SACLIB, noted that the reverse is also true, namely, that designing a system that someone else can plug-in is difficult. However, our symbolic software is becoming very complex and a solution to Problem 7 is crucial.

8. Killer Applications

The commercial success of a computer product is, according to Stephen Jobs, dependent on a so-called “killer” application that everyone wants but only the one product has. In Table 2 I attempt to list the killer app’s for several products, including symbolic software.

Certainly, the students learning calculus with the help of a computer algebra system constitute the most numerous users of our software. At North Carolina State University alone they number about 8000 per year. Such proliferation of use makes a discipline important to society, but it also influences the direction of its future development. I am told that much of the MathML Internet standard is geared towards mathematics education. My last problem, admittedly non-scientific, addresses this situation.

OPEN PROBLEM 8. Besides mathematics education, find another so-called “killer” application for symbolic computation.

The problem is solved when the new application makes the software written for it a commercial success.

Summary, Acknowledgement and Note Added in March 2000

These are my open problems.

- (1) Nearby multivariate polynomials that factor over \mathbb{C} .

- (2) Zolotarev's problem on a computer.
- (3) Characteristic polynomial of a black box matrix.
- (4) Lattice basis reduction-safe GGH-like cryptosystems.
- (5) Gröbner bases via iterative numerical methods.
- (6) Space and time efficient transposition principle.
- (7) Plug-and-play and generic programming methodology for symbolic computation.
- (8) Another "killer" application besides education.

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The above problems were posed in April 1998. To my knowledge, none has been resolved as of March 2000. However, there has been significant progress on several of them, which I would like to mention. Problem 1 has been tackled by several authors using numerical techniques. While the resulting algorithms do not resolve the problem in its entirety, the solutions are nonetheless useful in many cases, similarly to complex root finding procedures that do not converge for all inputs. Good progress can be reported on problem 3. Gilles Villard has found an algorithm that is within a factor of $n^{1/2+o(1)}$ of the required complexity. The algorithm does not rely on fast matrix multiplication algorithms and therefore is more practical than those methods, which are still asymptotically faster. Important research is being conducted on problem 7, but I shall only provide some references (Bernardin *et al.*, 1999; Le and Howlett, 1999; Wang, 1999). The solution of problem 8 may lie in the past. The Nobel Prize in physics was awarded in 1999 to Gerardus 't Hooft and Martinus J. G. Veltman, and as the citation of the Nobel Foundation reads [www.nobel.se/announcement-99/physics99.html] "At the end of the 1960s . . . Veltman had developed the Schoonschip computer program which, using symbols, performed algebraic simplifications of the complicated expressions that all quantum field theories result in when quantitative calculations are performed. . . . With the help of Veltman's computer program 't Hooft's partial results were now verified and together they worked out a calculation method in detail."

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Appendix A. Complex Variables in Computer Algebra (by R. M. Corless and D. J. Jeffrey)

By now, many users and most developers of computer algebra systems (CAS) are familiar with a set of problems known generically for many years as “the square root bug.” What was meant by this expression was that CAS would sometimes transform complex-valued expressions incorrectly. The example that gave the bug its name was the transformation of $\sqrt{x^2}$ to x , which is not even valid for all real x , much less for complex x . Squarely at the root of the difficulty is multivaluedness, which does happen with real variables, but is much more common with complex variables.

A concise and elegant description of the problem can be found in Stoutemyer (1991). More discussion can be found in the papers by Aslaksen, by Patton, by Fateman, by Rich and Jeffrey, and by Corless and Jeffrey in Issue 116 (June 1996) of the ACM SIGSAM BULLETIN (Communications in Computer Algebra).

One of the fundamental difficulties in dealing with “the square root bug” is that because of multivaluedness, some cherished algebraic identities, such as

$$\ln z_1 z_2 = \ln z_1 + \ln z_2, \tag{A1}$$

no longer hold—they are not true for all specializations of the variables. People have been willing to try to keep these identities, at almost any cost. For example, in Carathéodory (1964), even Carathéodory was willing to change the meaning of equality in order to keep equation (A1). He changed the interpretation of the symbols in the formula in two ways. First, he interpreted each side as a set. Second, he interpreted the equals sign to mean that the set represented on the left-hand side of the equals sign had a non-empty intersection with the set represented on the right-hand side. [†] In a discussion at ECCAD

[†]Note added in proof: Unlike the English translation, Carathéodory’s original German version of this passage does not lend itself to this interpretation, but rather to set equality (observation courtesy A. Davenport). However, even so, set equality of $\ln z_1 z_2$ and $\ln z_1 + \ln z_2$ does not imply set equality of $\ln z^2$ and $2 \ln z$, because of correlations (observation courtesy J. H. Davenport).

'98, Dana Scott observed that Carathéodory's notion of equality is not transitive, and hence is not an equivalence relation.

Other approaches, such as Riemann surfaces, are also not satisfactory (chiefly because algebra on them seems so difficult).

One of the main consequences of these mathematical difficulties is that there have been persistent bugs in many computer algebra systems, particularly in integration, where changing interpretations of square roots or the like have resulted in absurdities such as positive integrands giving negative (definite) integrals. It is a firmly held conviction in CAS that the proper setting for the integration problem is the complex plane. One consequence is that it is quite possible to integrate f' to obtain $f+c$ where c is a complex piecewise constant; indeed the discontinuities in c may be complex.

While we would like to pose the general problem of correct simplification of complex-valued transcendental functions as our "open problem", we feel that this is both too vague and too difficult. On the other hand, "fixing all the bugs in CAS" does not have the right tone either. Instead, we focus on a smaller subproblem in this area.

Recent progress on "the square root bug" includes the removal by all major computer algebra systems of automatic simplifications that are not always true on specialization over the complex numbers (except possibly on sets of measure zero). Progress has also been made on integration, particularly with the papers of Jeffrey (1993, 1994, 1997) and Jeffrey and Rich (1994). The main contribution of these papers is that it is better to return an integral that is continuous on a domain of maximum extent, rather than trying to fix up spurious singularities and branch cuts later. See also a discussion of Rioboo's algorithm, such as the one in Bronstein (1997).

However, these papers address only the simplest sorts of integrals. One of the central pillars of computer algebra is the Risch integration algorithm and its extensions (see, for example, Bronstein, 1997). The algorithm, which is algebraic and not analytic in its essentials, does not always produce integrals continuous on domains of maximum extent. Further, it often forces computation into the complex plane. For a simple example, consider the following Maple session.

```
> infolevel[int] := 5;
```

$$\text{infolevel}_{int} := 5.$$

We force Maple to skip its inexpensive heuristics and go to the Risch algorithm, normally a last resort.

```
> ah := 'int/risch_like'(1/(2+sin(z)),z);
```

```
int/risch: enter Risch integration
```

```
int/risch/algebraic1: RootOfs should be algebraic numbers and functions
```

```
int/risch: the field extensions are
```

$$[z, e^{(\text{RootOf}(-Z^2+1)z)}]$$

```
int/risch: Introduce the namings:
```

$$\{-th_1 = e^{(\text{RootOf}(-Z^2+1)z)}\}$$

```
unknown: integrand is
```

$$\frac{1}{2 - \frac{1}{2} \operatorname{RootOf}(-Z^2 + 1) \left(-th_1 - \frac{1}{-th_1} \right)}$$

unknown: integrand expressed as

$$2 \frac{\operatorname{RootOf}(-Z^2 + 1) - th_1}{4 \operatorname{RootOf}(-Z^2 + 1) - th_1 + -th_1^2 - 1}$$

int/risch/ratpart: integrating

$$2 \frac{\operatorname{RootOf}(-Z^2 + 1) - th_1}{4 \operatorname{RootOf}(-Z^2 + 1) - th_1 + -th_1^2 - 1}$$

int/risch/ratpart: Hermite reduction yields

$$\int 2 \frac{\operatorname{RootOf}(-Z^2 + 1) - th_1}{4 \operatorname{RootOf}(-Z^2 + 1) - th_1 + -th_1^2 - 1} dz$$

int/risch/ratpart: Rothstein's method - factored resultant is

$$3z^2 + 1$$

int/risch/ratpart: result is

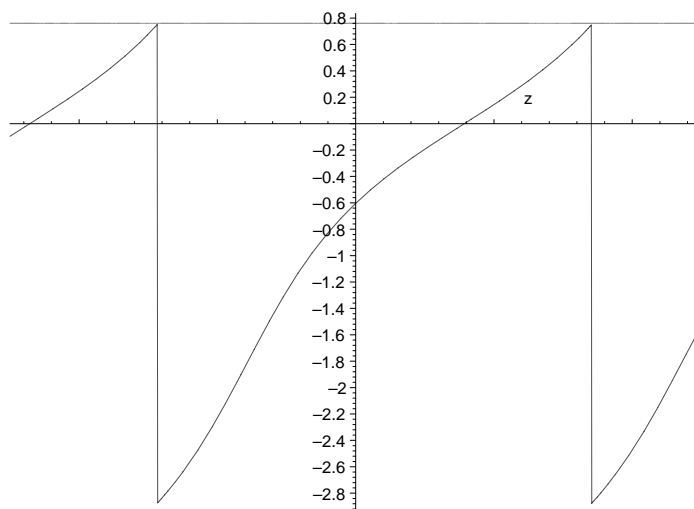
$$\frac{1}{3} I \sqrt{3} \ln(-th_1 + I \sqrt{3} + 2 \operatorname{RootOf}(-Z^2 + 1)) - \frac{1}{3} I \sqrt{3} \ln(-th_1 - I \sqrt{3} + 2 \operatorname{RootOf}(-Z^2 + 1))$$

int/risch: exit Risch integration

$$ah := \frac{1}{3} I \sqrt{3} \ln(e^{(Iz)} + I \sqrt{3} + 2I) - \frac{1}{3} I \sqrt{3} \ln(e^{(Iz)} - I \sqrt{3} + 2I).$$

We see by the following plot that the Risch algorithm applied to this simple problem does not produce a continuous antiderivative.

```
> plot([evalc(Re(ah)), evalc(Im(ah))], z=-5..5);
```



OPEN PROBLEM 9. Modify (or replace) the Risch algorithm so as to produce integrals continuous on domains of maximum extent, or else clearly describe the largest class of functions (elementary or other) for which continuous antidifferentiation can be done efficiently.

This problem will be known to be solved when a proof of the algorithm's correctness appears in a good journal, or more preferably when the algorithm is implemented in a major CAS and thus made available for general use and scrutiny.

Since, even for the integration of rational functions over a complex field, we can have branch cuts consisting of any algebraic curve whatsoever, this seems difficult. For rational functions over a real field, Rioboo's algorithm can be used (Bronstein, 1997). Some related issues include the following.

APPENDIX A.1. DOMAINS OF COMPUTATION

We feel that the default domain of computation should match the user's expectations (and be modifiable at the user's will). If the computer algebra system begins its computations in the real domain, assuming all variables are real and all functions are real-valued, then if at any time during the computation the system decides to move into the complex domain, as it did in our Risch example, then the user should be warned somehow; B. F. Caviness has suggested that the background colour of the screen could change, for example.

Automatic simplifications should only perform transformations valid for all specializations of the variables in the domain in question (possibly using dynamic evaluation, or provisos). The user, of course, should be allowed to perform any manipulation she or he desires.

APPENDIX A.2. INTEGRATION OF SPECIAL FUNCTIONS

There are several classes of complex-valued special functions which are of great value to the scientist, not all of which are supported equally well by the major computer algebra systems. Examples include the Jacobian elliptic functions and elliptic integrals, and the hypergeometric or even Meijer G functions or still more generally the so-called "H-functions". The Jacobian elliptic functions are very rich in algebraic identities, occur very often in applications (see the beautiful book Lawden, 1989), and being doubly-periodic in the complex plane have multivalued inverses. Therefore, all the difficulties talked about earlier are inherited here as well.

As an example, consider

$$\int \operatorname{cn}(u, k) \, du . \tag{A2}$$

We will use the substitution $\phi = \operatorname{am}(u)$, where $\operatorname{am}(u)$ is Jacobi's amplitude function and satisfies

$$\begin{aligned} \operatorname{sn}(u, k) &= \sin(\operatorname{am}(u, k)) = \sin(\phi) \\ \operatorname{cn}(u, k) &= \cos(\operatorname{am}(u, k)) = \cos(\phi) \\ \frac{d}{du} \operatorname{am}(u, k) &= \operatorname{dn}(u, k) . \end{aligned}$$

This gives that $du = d\phi/\sqrt{1 - k^2 \sin^2 \phi}$, on using the identity

$$k^2 \operatorname{sn}^2(u, k) + \operatorname{dn}^2(u, k) = 1.$$

Therefore, we may express any integrand rational in sn , cn , and dn as an algebraic integral in $\sin(\phi)$ and $\cos(\phi)$ by a simple change of variables. Our simple example gives

$$\int \operatorname{cn}(u, k) du = \int \frac{\cos(\phi) d\phi}{\sqrt{1 - k^2 \sin^2(\phi)}}. \quad (\text{A3})$$

It is an easy exercise (Lawden, 1989, p. 40) to show that this is in fact equal to $\int \operatorname{cn}(u, k) du = \sin^{-1}(k \operatorname{sn}(u, k))/k$, up to a constant. More interestingly, Maple gives a non-trivial discontinuous integral for the following continuous integrand (with explicit use of `changevar`, because otherwise Maple does not know how to integrate the Jacobian elliptic functions as yet):

$$\int \frac{du}{2 + \operatorname{cn}(u, k)} = \int \frac{d\phi}{(2 + \cos \phi) \sqrt{1 - k^2 \sin^2 \phi}}. \quad (\text{A4})$$

We leave the verification of this as an exercise for the reader.

Integration of all these functions would be very useful; integration valid on domains of maximum extent would be more useful. Although the simplification of expressions containing these functions and a few transcendental constants is impossible in general (even recognizing zero is undecidable),[†] one can still ask packages to do as much as is possible.

APPENDIX A.3. BRANCHES AND THE UNWINDING NUMBER

Many people have tried to automate symbolic computations with multivalued functions; see, for example, Dingle and Fateman (1994) or Corless and Jeffrey (1996). It now appears, at least for the logarithm and hence for simple elementary functions, that complex analysis can be turned into computer algebra. Once you replace the (false) identity $\ln \exp z = z$ with the true identity

$$\ln e^z = z - 2\pi i \mathcal{K}(z), \quad (\text{A5})$$

where \mathcal{K} is the so-called “unwinding number”, then computer algebra systems can manipulate some complex formulæ correctly. The geometric information about the branch cuts is encoded in the arguments to the unwinding number (which makes this approach similar, in fact, to that of Dingle and Fateman, 1994). There are simple theorems one can use to simplify some unwinding numbers, and other algebraic identities that can be

[†]As a point of clarification, it is useful to emphasize the distinction between the undecidability of algebraic simplification in general and the decidability of integration once the model for the field of extensions is known, as shown by Risch. See Bronstein (1997) for a detailed discussion.

implemented, such as

$$\begin{aligned}\mathcal{K}(z) &= \left\lceil \frac{\operatorname{Im}(z) - \pi}{2\pi} \right\rceil \\ \ln z_1 z_2 &= \ln z_1 + \ln z_2 - 2\pi i \mathcal{K}(\ln z_1 + \ln z_2) \\ w \ln z &= \ln z^w + 2\pi i \mathcal{K}(w \ln z) \\ \mathcal{K}(z + 2\pi i n) &= \mathcal{K}(z) + n \\ \mathcal{K}(\ln z) &= 0 \\ z_1^w z_2^w &= (z_1 z_2)^w \exp(2\pi i w \mathcal{K}(\ln z_1 + \ln z_2)) \\ z^{vw} &= (z^v)^w \exp(2\pi i v w \mathcal{K}(v \ln z)).\end{aligned}$$

A prototype implementation in Maple is under construction, by Gurjeet Litt (a Masters' student at the University of Western Ontario at this time of writing).

The talk from which the material of this appendix was extracted can be found at <http://www.apmaths.uwo.ca/~rmc/papers/symbolic/index.html> under the heading "East Coast Computer Algebra Day 1998."

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