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'PSLQ Algorithm' A New Approach in Mathematics Experimental

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***Abstract:* While extensive usage of high-performance computing has been a staple of other scientific and engineering disciplines for some time, research mathematics is one discipline that has heretofore not yet benefited to the same degree. Now, however, with sophisticated mathematical computing tools and environments widely available on desktop computers, a growing number of remarkable new mathematical results are being discovered partly or entirely with the aid of these tools. For many years, researchers have dreamed of a facility that permits one to recognize a numeric constant in terms of the mathematical formula that it satisfies. With the advent of efficient integer relation detection algorithms, that time has arrived. This article briefly discusses the nature of the mathematical experiment. It then presents a few instances primarily of our own recent computer-aided mathematical discoveries and sketches the outlook for the future.**

***Keywords:* Algebraic Relations, Algorithm.**

PRELIMINARIES

The crucial role of high-performance computing is now acknowledged throughout the physical, biological and engineering sciences. Numerical experimentation, using increasingly large-scale, three-dimensional simulation programs, is now a staple of fields such as aeronautical and electrical engineering, and research scientists heavily utilize computing technology to collect and analyze data, and to explore the implications of various physical theories. However, "pure" mathematics only recently has begun to capitalize on this new technology.

INTRODUCTION

The most obvious development in mathematical computing technology has been the growing availability of powerful symbolic computing tools. A recent development that has been key to a number of new discoveries is the emergence of practical integer relation detection algorithms. Let $x = (x_1, x_2, \cdot \cdot \cdot, x_n)$ be a vector of real or complex numbers. x is said to possess an integer relation if there exist integers a_i, not all zero, such that $a_1x_1 + a_2x_2 + \cdot \cdot \cdot + a_nx_n = 0$.
By an *integer relation algorithm*, we mean a practical computational scheme that can recover the vector of integers a_i, if it exists, or can produce bounds within which no integer relation exists. As we shall see, integer relation algorithms have a variety of interesting applications, including the recognition of a numeric constant in terms of the mathematical formula that it satisfies
At the present time, the most effective scheme for integer relation detection is Ferguson's "PSLQ" algorithm. The name "PSLQ" derives from its usage of a partial sum of squares vector and a LQ (Lower-diagonal-orthogonal) matrix factorization.

A NEW FORMULA FOR Pi

Through the centuries mathematicians have assumed that there is no shortcut to determining just the n^{th} digit of π. Thus it came as no small Surprise when such a scheme was recently discovered. In particular, this simple algorithm allows one to calculate the n-th hexadecimal digit of π without computing any of the first $n-1$ digits, without the need for multiple-precision arithmetic software and requiring only a very small amount of memory. The one millionth hex digit of π can be computed in this manner on a current-generation personal computer in only about 30 seconds run time. This scheme is based on the following remarkable formula,

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k} \left[\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right]$$

This formula was found using months of PSLQ computations, after corresponding but simpler *n*-th digit formulas were identified for several other constants, including log(2).
Similar base-2 formulas are given for a number of other mathematical constants. Some base-3 formulas were obtained, including the identity

$$\pi^2 = \frac{2}{27}\sum_{k=0}^{\infty}\frac{1}{729^k}\left[\frac{243}{(12k+1)^2} - \frac{405}{(12k+2)^2} - \frac{81}{(12k+4)^2} - \frac{27}{(12k+5)^2} - \frac{72}{(12k+6)^2} - \frac{9}{(12k+7)^2} - \frac{9}{(12k+8)^2} - \frac{5}{(12k+10)^2} + \frac{1}{(12k+11)^2}\right]$$

FINDING ALGEBRAIC RELATIONS

One application of PSLQ in the field of mathematical number theory is to determine whether or not a given constant α, whose value can be computed to high precision, is algebraic of some degree n or less. This can be done by first computing the vector $x = (1, \alpha_1, \alpha_2, \cdot\ \cdot\ \cdot, \alpha_n)$ to high precision and then applying an integer relation algorithm. If a relation is found for x, then this relation vector is precisely the set of integer coefficients of a polynomial satisfied by α. Even if no relation is found integer relation detection programs can produce bounds within which no relation can exist.

IDENTITIES FOR THE RIEMANN ZETA FUNCTION

Consider, for example, the following identities:

$$\zeta(2) = 3\sum_{k=1}^{\infty}\frac{1}{k^2\binom{2k}{k}}$$

$$\zeta(3) = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k^3\binom{2k}{k}}$$

$$\zeta(4) = \frac{36}{17}\sum_{k=1}^{\infty}\frac{1}{k^4\binom{2k}{k}}$$

where $\zeta(n) = \sum_k k^{-n}$ is the Riemann zeta function at n. These results have led many to hope that

$$Z_5 = \zeta(5)/\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k^5\binom{2k}{k}} \qquad (1)$$

Might also be a simple rational or algebraic number. However, computations using PSLQ established, for instance, that if Z_5 satisfies a polynomial of degree 25 or less, then the Euclidean norm of the coefficients must exceed 2×10^{37}.

A NOTE OF CAUTION

In spite of the remarkable successes of this methodology, some caution is in order. First of all, the fact that an identity is established to high precision is *not* a guarantee that it is indeed true. One example is

$$\sum_{n=1}^{\infty}\frac{[n\tanh\pi]}{10^n} \approx \frac{1}{81}$$

Which holds to 267 digits, yet is not an exact identity, failing in the 268'Th place.
More generally speaking, caution must be exercised when extrapolating results true for small *n* to all *n*. For example,

$$\int_0^\infty \frac{\sin(x)}{x}\,dx = \frac{\pi}{2}$$

$$\int_0^\infty \frac{\sin(x)}{x}\frac{\sin(x/3)}{x/3}\,dx = \frac{\pi}{2}$$

$$\cdots$$

$$\int_0^\infty \frac{\sin(x)}{x}\frac{\sin(x/3)}{x/3}\cdots\frac{\sin(x/13)}{x/13}\,dx = \frac{\pi}{2}$$

yet

$$\int_0^\infty \frac{\sin(x)}{x}\frac{\sin(x/3)}{x/3}\cdots\frac{\sin(x/15)}{x/15}\,dx = \frac{467807924713440738696537864469}{935615849440640907310521750000}\pi.$$

When this fact was recently observed by a researcher using a mathematical software package, he concluded that there must be a "bug" in the software. Not so. What is happening here is that

$$\int_0^\infty \frac{\sin(x)}{x}\frac{\sin(x/h_1)}{x/h_1}\cdots\frac{\sin(x/h_n)}{x/h_n}\,dx = \frac{\pi}{2}$$

only so long as $1/h_1 + 1/h_2 + \cdot\cdot\cdot + 1/h_n < 1$. In the above example, $1/3 + 1/5 + \cdot\cdot\cdot + 1/13 < 1$, but with the addition of 1/15, the sum exceeds 1 and the identity no longer holds. Changing the h_n lets this pattern persist indefinitely but still fail in the large.

FUTURE OUTLOOK

Computer mathematics software is now becoming a staple of university departments and government research laboratories. Many university departments now offer courses where the usage of one of these software packages is an integral part of the course. But further expansion of these facilities into high schools has been inhibited by a number of factors, including the fairly high cost of such software, the lack of appropriate computer equipment, difficulties in standardizing such coursework at a regional or national level, a paucity of good texts incorporating such tools into a realistic curriculum, lack of trained teachers and many other demands on their time. But computer hardware continues its downward spiral in cost and its upward spiral in power. It thus appears that within very few years, moderately powerful symbolic computation facilities can be incorporated into relatively inexpensive hand calculators, at which point it will be much easier to successfully integrate these tools into high school curricula. Thus it seems that we are poised to see a new generation of students coming into university mathematics and science programs who are completely comfortable using such tools. This development is bound to have a profound impact on the future teaching, learning and doing of mathematics.

A likely and fortunate spin-off of this development is that the commercial software vendors who produce these products will likely enjoy a broader financial base, from which they can afford to further enhance their products geared at serious researchers. Future enhancements are likely to include more efficient algorithms, more extensive capabilities mixing numerics and symbolics, more advanced visualization facilities, and software optimized for emerging symmetric multiprocessor and highly parallel, distributed memory computer systems. We only now are beginning to experience and comprehend the potential impact of computer mathematics tools on mathematical research. In ten more years, a new generation of computer-literate mathematicians, armed with significantly improved software on prodigiously powerful computer systems, are bound to make discoveries in mathematics that we can only dream of at the present time.

CONCLUSION

We have shown a small but we hope the convincing selection of what the present allows and what the future holds in store. We have hardly mentioned the growing ubiquity of web-based computation, or of pervasive access to massive databases, both public domain, and commercial. Neither have we raised the human/computer interface or intellectual property issues and the myriad other not-purely-technical issues these raise.

Whatever the outcome of these developments, we are still persuaded that mathematics is and will remain a uniquely human undertaking. One could even argue that these developments confirm the fundamentally human nature of mathematics. Indeed, for a humanist philosophy of mathematics, as paraphrased below, become more convincing in our setting:

1. Mathematics is human. It is part of and fits into human culture.
2. Mathematical knowledge is fallible. As in science, mathematics can advance by making mistakes and then correct or even re-correcting them.
3. There are different versions of proof or rigor.
4. Empirical evidence, numerical experimentation and probabilistic proof all can help us decide what to believe in mathematics.
5. Mathematical objects are a special variety of a social-cultural-historical object. Contrary to the assertions of certain postmodern detractors, mathematics cannot be dismissed as merely a new form of literature or religion. Nevertheless, many mathematical objects can be seen as shared ideas. Certainly, the recognition that "quasi-intuitive" analogies can be used to gain insight in mathematics can assist in the learning of mathematics. And honest mathematicians will acknowledge their role in discovery as well. We look forward to what the future will bring.

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