MULTIPLE-PRECISION ZERO-FINDING METHODS AND THE COMPLEXITY OF ELEMENTARY FUNCTION EVALUATION

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ABSTRACT

We consider methods for finding high-precision approximations to simple zeros of smooth functions. As an application, we give fast methods for evaluating the elementary functions $\log(x)$, $\exp(x)$, $\sin(x)$ etc. to high precision. For example, if x is a positive floating-point number with an n-bit fraction, then (under rather weak assumptions) an n-bit approximation to $\log(x)$ or $\exp(x)$ may be computed in time asymptotically equal to $13M(n)\log_2 n$ as $n \to \infty$, where $M(n)$ is the time required to multiply floating-point numbers with n-bit fractions. Similar results are given for the other elementary functions, and some analogies with operations on formal power series are mentioned.

1. INTRODUCTION

When comparing methods for solving nonlinear equations or evaluating functions, it is customary to assume that the basic arithmetic operations (addition, multiplication, etc.) are performed with some fixed precision. However, an irrational number can only be approximated to arbitrary accuracy if the precision is allowed to increase indefinitely. Thus, we shall consider iterative processes using variable precision. Usually

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the precision will increase as the computation proceeds, and the final result will be obtained to high precision. Of course, we could use the same (high) precision throughout, but then the computation would take longer than with variable precision, and the final result would be no more accurate.

Assumptions

For simplicity we assume that a standard multiple-precision floating-point number representation is used, with a binary fraction of n bits, where n is large. The exponent length is fixed, or may grow as $o(n)$ if necessary. To avoid table-lookup methods, we assume a machine with a finite random-access memory and a fixed number of sequential tape units. Formally, the results hold for multitape Turing machines.

Precision n Operations

An operation is performed with precision n if the operands and result are floating-point numbers as above (i.e., precision n numbers), and the relative error in the result is $0(2^{-n})$.

Precision n Multiplication

Let $M(n)$ be the time required to performe precision n multiplication. (Time may be regarded as the number of single-precision operations, or the number of bit operations, if desired.) The classical method gives $M(n) = 0(n^2)$, but methods which are faster for large n are known. Asymptotically the fastest method known is that of Schönhage and Strassen [71], which gives

$$M(n) = 0(n.\log(n)\log\log(n)) \quad \text{as} \quad n \to \infty. \tag{1.1}$$

Our results do not depend on the algorithm used for multiplication, provided $M(n)$ satisfies the following two conditions.

(1.2) $\quad n = o(M(n))$, i.e., $\lim_{n\to\infty} n/M(n) = 0$;

and, for any $\alpha > 0$,

(1.3) $\quad M(\alpha n) \sim \alpha M(n)$, i.e., $\lim_{n\to\infty} \frac{M(\alpha n)}{\alpha M(n)} = 1$.

Condition (1.2) enables us to neglect additions, since the time for an addition is $O(n)$, which is asymptotically negligible compared to the time for a multiplication. Condition (1.3) certainly holds if

$$M(n) \sim cn[\log(n)]^{\beta}[\log\log(n)]^{\gamma} ,$$

though it does not hold for some implementations of the Schönhage-Strassen method. We need (1.3) to estimate the constants in the asymptotic "O" results: if the constants are not required then much weaker assumptions suffice, as in Brent [75a,b].

The following lemma follows easily from (1.3).

Lemma 1.1

If $0 < \alpha < 1$, $M(n) = 0$ for $n < 1$, and $c_1 < \frac{1}{1-\alpha} < c_2$, then

$$c_1 M(n) < \sum_{k=0}^{\infty} M(\alpha^k n) < c_2 M(n)$$

for all sufficiently large n .

2. BASIC MULTIPLE-PRECISION OPERATIONS

In this section we summarize some results on the time required to perform the multiple-precision operations of division, extraction of square roots, etc. Additional results are given in Brent [75a].

Reciprocals

Suppose $a \neq 0$ is given and we want to evaluate a precision n approximation to $1/a$. Applying Newton's method to the equation

$$f(x) \equiv a - 1/x = 0$$

gives the well-known iteration

$$x_{i+1} = x_i - x_i\varepsilon_i ,$$

where

$$\varepsilon_i = ax_i - 1 .$$

Since the order of convergence is two, only $k \sim \log_2 n$ iterations are required if x_0 is a reasonable approximation to $1/a$, e.g., a single-precision approximation.

If $\varepsilon_k = 0(2^{-n})$, then $\varepsilon_{k-1} = 0(2^{-n/2})$, so at the last iteration it is sufficient to perform the multiplication of x_{k-1} by ε_{k-1} using precision $n/2$, even though ax_{k-1} must be evaluated with precision n. Thus, the time required for the last iteration is $M(n) + M(n/2) + 0(n)$. The time for the next to last iteration is $M(n/2) + M(n/4) + 0(n/2)$, since this iteration need only give an approximation accurate to $0(2^{-n/2})$, and so on. Thus, using Lemma 1.1, the total time required is

$$I(n) \sim (1 + \tfrac{1}{2})(1 + \tfrac{1}{2} + \tfrac{1}{4} + \ldots)M(n) \sim 3M(n)$$

as $n \to \infty$.

Division

Since $b/a = b(1/a)$, precision n division may be done in time

$$D(n) \sim 4M(n)$$

as $n \to \infty$.

Inverse Square Roots

Asymptotically the fastest known method for evaluating $a^{-\frac{1}{2}}$ to precision n is to use the third-order iteration

$$x_{i+1} = x_i - \tfrac{1}{2}x_i(\varepsilon_i - \tfrac{3}{4}\varepsilon_i^2) ,$$

where

$$\varepsilon_i = ax_i^2 - 1 .$$

At the last iteration it is sufficient to evaluate ax_i^2 to precision n, ε_i^2 to precision $n/3$, and $x_i(\varepsilon_i - \frac{3}{4}\varepsilon_i^2)$ to precision $2n/3$. Thus, using Lemma 1.1 as above, the total time required is

$$Q(n) \sim (2 + \tfrac{1}{3} + \tfrac{2}{3})(1 + \tfrac{1}{3} + \tfrac{1}{9} + \ldots)M(n) \sim 4\tfrac{1}{2}M(n)$$

as $n \to \infty$.

Square Roots

Since

$$a^{\frac{1}{2}} = \begin{cases} a.a^{-\frac{1}{2}} & \text{if } a > 0 , \\ 0 & \text{if } a = 0 , \end{cases}$$

we can evaluate $a^{\frac{1}{2}}$ to precision n in time

$$R(n) \sim 5\tfrac{1}{2}M(n)$$

as $n \to \infty$. Note that the direct use of Newton's method in the form

(2.1) $$x_{i+1} = \tfrac{1}{2}(x_i + a/x_i)$$

or

(2.2) $$x_{i+1} = x_i + \left(\frac{a - x_i^2}{2x_i}\right)$$

is asymptotically slower, requiring time $\sim 8M(n)$ or $\sim 6M(n)$ respectively.

3. VARIABLE-PRECISION ZERO-FINDING METHODS

Suppose $\zeta \neq 0$ is a simple zero of the nonlinear equation

$$f(x) = 0 .$$

Here, $f(x)$ is a sufficiently smooth function which can be evaluated near ζ, with absolute error $0(2^{-n})$, in time $w(n)$. We consider some methods for evaluating ζ to precision n.

Since we are interested in results for very large n, the time required to obtain a good starting approximation is neglected.

Assumptions

To obtain sharp results we need the following two assumptions, which are similar to (1.2) and (1.3):

(3.1) $\quad M(n) = o(w(n))$, i.e., $\lim_{n\to\infty} M(n)/w(n) = 0$;

and, for some $\alpha \geq 1$ and all $\beta > 0$,

(3.2) $$w(\beta n) \sim \beta^{\alpha} w(n)$$

as $n \to \infty$.

From (3.1), the time required for a multiplication is negligible compared to the time for a function evaluation, if n is sufficiently large. (3.2) implies (3.1) if $\alpha > 1$, and (3.2) certainly holds if, for example,

$$w(n) \sim cn^{\alpha}[\log(n)]^{\gamma}[\log\log(n)]^{\delta} .$$

The next lemma follows from our assumptions in much the same way as Lemma 1.1.

Lemma 3.1

If $0 < \beta < 1$, $w(n) = 0$ for $n < 1$, and

$$c_1 < 1/(1 - \beta^{\alpha}) < c_2 ,$$

then

$$c_1 w(n) < \sum_{k=0}^{\infty} w(\beta^k n) < c_2 w(n)$$

for all sufficiently large n .

A Discrete Newton Method

To illustrate the ideas of variable-precision zero-finding methods, we describe a simple discrete Newton method. More efficient methods are described in the next three sections, and

in Brent [75a].

Consider the iteration

$$x_{i+1} = x_i - f(x_i)/g_i ,$$

where g_i is a one-sided difference approximation to $f'(x_i)$, i.e.,

$$g_i = \frac{f(x_i + h_i) - f(x_i)}{h_i} .$$

If $\varepsilon_i = |x_i - \zeta|$ is sufficiently small, $f(x_i)$ is evaluated with absolute error $0(\varepsilon_i^2)$, and h_i is small enough that

$$g_i = f'(x_i) + 0(\varepsilon_i) , \tag{3.3}$$

then the iteration converges to ζ with order at least two. To ensure (3.3), take h_i of order ε_i, e.g. $h_i = f(x_i)$.

To obtain ζ to precision n, we need two evaluations of f with absolute error $0(2^{-n})$, preceded by two evaluations with error $0(2^{-n/2})$, etc. Thus, the time required is

$$t(n) \sim 2(1 + 2^{-\alpha} + 2^{-2\alpha} + \ldots)w(n) . \tag{3.4}$$

Asymptotic Constants

We say that a zero-finding method has asymptotic constant $C(\alpha)$ if, to find a simple zero $\zeta \neq 0$ to precision n, the method requires time $t(n) \sim C(\alpha)w(n)$ as $n \to \infty$. (The asymptotic constant as defined here should not be confused with the "asymptotic error constant" as usually defined for single-precision zero-finding methods.)

For example, from (3.4), the discrete Newton method described above has asymptotic constant

$$C_N(\alpha) = 2/(1 - 2^{-\alpha}) \leq 4 .$$

Note that the time required to evaluate ζ to precision n is only a small multiple of the time required to evaluate $f(x)$

with absolute error $0(2^{-n})$. (If we used fixed precision, the time to evaluate ζ would be $0(\log(n))$ times the time to evaluate $f(x)$.)

4. A VARIABLE-PRECISION SECANT METHOD

The secant method is known to be more efficient than the discrete Newton method when fixed-precision arithmetic is used. The same is true with variable-precision arithmetic, although the ratio of efficiencies is no longer constant, but depends on the exponent α in (3.2). Several secant-like methods are described in Brent [75a]; here we consider the simplest such method, which is also the most efficient if $\alpha < 4.5243...$.

The secant iteration is

$$x_{i+1} = x_i - f_i \left[\frac{x_i - x_{i-1}}{f_i - f_{i-1}}\right] ,$$

where $f_i = f(x_i)$, and we assume that the function evaluations are performed with sufficient accuracy to ensure that the order of convergence is at least $\rho = \frac{1}{2}(1 + 5^{\frac{1}{2}}) = 1.6180...$, the larger root of

$$\rho^2 = \rho + 1 . \tag{4.1}$$

Let $\varepsilon = |x_{i-1} - \zeta|$. Since the smaller root of (4.1) lies inside the unit circle, we have

$$x_i - \zeta = 0(\varepsilon^{\rho})$$

and

$$x_{i+1} - \zeta = 0(\varepsilon^{\rho^2}) .$$

To give order ρ , f_i must be evaluated with absolute error $0(\varepsilon^{\rho^2})$. Since $f_i = 0(|x_i - \zeta|) = 0(\varepsilon^{\rho})$, it is also necessary to evaluate $(f_i - f_{i-1})/(x_i - x_{i-1})$ with relative error $0(\varepsilon^{\rho^2 - \rho})$, but $|x_i - x_{i-1}| \sim \varepsilon$, so it is necessary to evaluate f_{i-1} with absolute error $0(\varepsilon^{\rho^2 - \rho + 1})$. [Since

f_i must be evaluated with absolute error $0(\varepsilon^{\rho^2})$, f_{i-1} must be evaluated with absolute error $0(\varepsilon^{\rho})$, but $\rho^2 - \rho + 1 = 2 > \rho$, so this condition is superfluous.]

The conditions mentioned are sufficient to ensure that the order of convergence is at least ρ . Thus, if we replace ε^{ρ^2} by 2^{-n} , we see that ζ may be evaluated to precision n if f is evaluated with absolute errors $0(2^{-n})$, $0(2^{-2n\rho^{-2}})$, $0(2^{-2n\rho^{-3}})$, $0(2^{-2n\rho^{-4}})$, ... It follows that the asymptotic constant of the secant method is

$$C_S(\alpha) = 1 + (2\rho^{-2})^{\alpha}/(1 - \rho^{-\alpha}) \leq C_S(1) = 3 .$$

The following lemma states that the secant method is asymptotically more efficient than the discrete Newton method when variable precision is used.

Lemma 4.1

$C_S(\alpha) < C_N(\alpha)$ for all $\alpha \geq 1$. In fact, $C_S(\alpha)/C_N(\alpha)$ decreases monotonically from $\frac{3}{4}$ (when $\alpha = 1$) to $\frac{1}{2}$ (as $\alpha \to \infty$).

5. OTHER VARIABLE-PRECISION INTERPOLATORY METHODS

With fixed precision, inverse quadratic interpolation is more efficient than linear interpolation, and inverse cubic interpolation is even more efficient, if the combinatory cost (i.e., "overhead") is negligible. With variable precision the situation is different. Inverse quadratic interpolation is slightly more efficient than the secant method, but inverse cubic interpolation is not more efficient than inverse quadratic interpolation if $\alpha \lesssim 4.6056...$. Since the combinatory cost of inverse cubic interpolation is considerably higher than that of inverse quadratic interpolation, the inverse cubic method appears even worse if combinatory costs are significant.

Inverse Quadratic Interpolation

The analysis of variable-precision methods using inverse quadratic interpolation is similar to that for the secant method, so we only state the results. The order $\rho = 1.8392...$ is the positive root of $\rho^3 = \rho^2 + \rho + 1$. It is convenient to define $\sigma = 1/\rho = 0.5436...$ To evaluate ζ to precision n requires evaluations of f to (absolute) precision n, $(1 - \sigma + \sigma^2)n$, and $\sigma^j(1 - \sigma - \sigma^2 + 2\sigma^3)n$ for $j=0,1,2,...$ Thus, the asymptotic constant is

$$C_Q(\alpha) = 1 + (1 - \sigma + \sigma^2)^\alpha + (3\sigma^3)^\alpha/(1 - \sigma^\alpha)$$

$$\lesssim C_Q(1) = \tfrac{1}{2}(7 - 2\sigma - \sigma^2) = 2.8085... .$$

Lemma 5.1

$C_Q(\alpha) < C_S(\alpha)$ for all $\alpha \gtrsim 1$. In fact, $C_Q(\alpha)/C_S(\alpha)$ increases monotonically from $0.9361...$ (when $\alpha = 1$) to 1 (as $\alpha \to \infty$).

Inverse Cubic Interpolation, etc.

If $\mu = 0.5187...$ is the positive root of $\mu^4 + \mu^3 + \mu^2 + \mu = 1$, then the variable-precision method of order $1/\mu = 1.9275...$, using inverse cubic interpolation, has asymptotic constant

$$C_C(\alpha) = 1 + (1 - \mu + \mu^2)^\alpha + (1 - \mu - \mu^2 + 2\mu^3)^\alpha + (4\mu^4)^\alpha/(1 - \mu^\alpha)$$

$$\lesssim C_C(1) = (13 - 6\mu - 4\mu^2 - 2\mu^3)/3 = 2.8438... .$$

Note that $C_C(1) > C_Q(1)$. Variable-precision methods using inverse interpolation of arbitrary degree are described in Brent [75a]. Some of these methods are slightly more efficient than the inverse quadratic interpolation method if α is large, but inverse quadratic interpolation is the most efficient method known for $\alpha < 4.6056...$. In practice α

is usually 1, 1½ or 2.

An Open Question

Is there a method with asymptotic constant $C(\alpha)$ such that $C(1) < C_Q(1)$?

6. VARIABLE-PRECISION METHODS USING DERIVATIVES

In Sections 3 to 5 we considered methods for solving the nonlinear equation $f(x) = 0$, using only evaluations of f. Sometimes it is easy to evaluate $f'(x)$, $f''(x)$, ... once $f(x)$ has been evaluated, and the following theorem shows that it is possible to take advantage of this. For an application, see Section 10.

Theorem 6.1

If the time to evaluate $f(x)$ with an absolute error $O(2^{-n})$ is $w(n)$, where $w(n)$ satisfies conditions (3.1) and (3.2), and (for $k=1,2,\ldots$) the time to evaluate $f^{(k)}(x)$ with absolute error $O(2^{-n})$ is $w_k(n)$, where

$$w_k(n) = o(w(n))$$

as $n \to \infty$, then the time to evaluate a simple zero $\zeta \neq 0$ of $f(x)$ to precision n is

$$t(n) \sim w(n)$$

as $n \to \infty$.

Proof

For fixed $k \geq 1$, we may use a direct or inverse Taylor series method of order $k + 1$. The combinatory cost is of order $k.\log(k + 1).M(n)$ (see Brent and Kung [75]). From (3.1), this is $o(w(n))$ as $n \to \infty$. Thus,

$$\begin{aligned} t(n) &\leq [1 - (k + 1)^{-\alpha}]^{-1} w(n) + o(w(n)) \\ &\leq (1 + \frac{1}{k} + o(1))w(n) . \end{aligned}$$

For sufficiently large n, the "$c(1)$" term is less than $1/k$, so

$$t(n) \lesssim (1 + \frac{2}{k})w(n) .$$

Given $\varepsilon > 0$, choose $k \gtrsim 2/\varepsilon$. Then, for all sufficiently large n,

$$w(n) \lesssim t(n) \lesssim (1 + \varepsilon)w(n) ,$$

so $t(n) \sim w(n)$ as $n \to \infty$.

Corollary 6.1

If the conditions of Theorem 6.1 hold, $f:[a,b] \to I$, $f'(x) \neq 0$ for $x \in [a,b]$, and g is the inverse function of f, then the time to evaluate $g(y)$ with absolute error $O(2^{-n})$, for $y \in I$, is

$$w_g(n) \sim w(n)$$

as $n \to \infty$.

Note

Corollary 6.1 is optimal in the sense that, if $w_g(n) \sim cw(n)$ for some constant $c < 1$, then $w(n) \sim cw_g(n)$ by the same argument, so $w(n) \sim c^2 w(n)$, a contradiction. Hence, $c = 1$ is minimal.

7. THE ARITHMETIC-GEOMETRIC MEAN ITERATION

Before considering the multiple-precision evaluation of elementary functions, we recall some properties of the arithmetic-geometric (A-G) mean iteration of Gauss [1876]. Starting from any two positive numbers a_0 and b_0, we may iterate as follows:

$$a_{i+1} = \frac{1}{2}(a_i + b_i) \quad \text{(arithmetic mean)}$$

and

$$b_{i+1} = (a_i b_i)^{\frac{1}{2}} \quad \text{(geometric mean)}$$

for $i=0,1,\ldots$.

Second-order Convergence

The A-G mean iteration is of computational interest because it converges very fast. If $b_i \ll a_i$, then

$$b_{i+1}/a_{i+1} = \frac{2(b_i/a_i)^{\frac{1}{2}}}{1 + b_i/a_i} \simeq 2(b_i/a_i)^{\frac{1}{2}} ,$$

so only about $|\log_2(a_0/b_0)|$ iterations are required before a_i/b_i is of order 1. Once a_i and b_i are close together the convergence is second order, for if $b_i/a_i = 1 - \varepsilon_i$ then

$$\varepsilon_{i+1} = 1 - b_{i+1}/a_{i+1} = 1 - 2(1 - \varepsilon_i)^{\frac{1}{2}}/(2 - \varepsilon_i) = \varepsilon_i^2/8 + 0(\varepsilon_i^3) .$$

Limit of the A-G Mean Iteration

There is no essential loss of generality in assuming that $a_0 = 1$ and $b_0 = \cos\phi$ for some ϕ. If $a = \lim_{i\to\infty} a_i = \lim_{i\to\infty} b_i$, then

$$a = \frac{\pi}{2K(\phi)} , \tag{7.1}$$

where $K(\phi)$ is the complete elliptic integral of the first kind, i.e.,

$$K(\phi) = \int_0^{\pi/2} (1 - \sin^2\phi\sin^2\theta)^{-\frac{1}{2}}d\theta .$$

(A simple proof of (7.1) is given in Melzak [73].)

Also, if $c_0 = \sin\phi$, $c_{i+1} = a_i - a_{i+1}$ $(i=0,1,\ldots)$, then

$$\sum_{i=0}^{\infty} 2^{i-1}c_i^2 = 1 - \frac{E(\phi)}{K(\phi)} , \tag{7.2}$$

where $E(\phi)$ is the complete elliptic integral of the second kind, i.e.,

$$E(\phi) = \int_0^{\pi/2} (1 - \sin^2\phi\sin^2\theta)^{\frac{1}{2}}d\theta .$$

Both (7.1) and (7.2) were known by Gauss.

Legendre's Identity

For future use, we note the identity

$$K(\phi)E(\phi') + K(\phi')E(\phi) - K(\phi)K(\phi') = \tfrac{1}{2}\pi \,, \tag{7.3}$$

where $\phi + \phi' = \frac{1}{2}\pi$. (Legendre [11] proved by differentiation that the left side of (7.3) is constant, and the constant may be determined by letting $\phi \to 0$.)

8. FAST MULTIPLE-PRECISION EVALUATION OF π

The classical methods for evaluating π to precision n take time $O(n^2)$: see, for example, Shanks and Wrench [62]. Several methods which are asymptotically faster than $O(n^2)$ are known. For example, in Brent [75a] a method which requires time $O(M(n)\log^2(n))$ is described. From the bound (1.1) on $M(n)$, this is faster than $O(n^{1+\varepsilon})$ for any $\varepsilon > 0$.

Asymptotically the fastest known methods require time $O(M(n)\log(n))$. One such method is sketched in Beeler et al [72]. The method given here is faster, and does not require the preliminary computation of e .

The Gauss-Legendre method

Taking $\phi = \phi' = \pi/4$ in (7.3), and dividing both sides by π^2 , we obtain

$$[2K(\pi/4)E(\pi/4) - K^2(\pi/4)]/\pi^2 = \frac{1}{2\pi} \,. \tag{8.1}$$

However, from the A-G mean iteration with $a_0 = 1$ and $b_0 = 2^{-\frac{1}{2}}$, and the relations (7.1) and (7.2), we can evaluate $K(\pi/4)/\pi$ and $E(\pi/4)/\pi$, and thus the left side of (8.1). A division then gives π . (The idea of using (7.3) in this way occurred independently to Salamin [75] and Brent [75b].) After a little simplification, we obtain the following algorithm (written in pseudo-Algol):

```
A ← 1;  B ← 2^(-½);  T ← 1/4;  X ← 1;
while  A - B > 2^(-n)  do
      begin  Y ← A;  A ← ½(A + B);  B ← (BY)^½;
             T ← T - X(A - Y)^2;
             X ← 2X
      end;
return  A^2/T  [or, better, (A + B)^2/(4T)] .
```

The rate of convergence is illustrated in Table 8.1.

Table 8.1: Convergence of the Gauss-Legendre Method

Iteration	$A^2/T - \pi$	$\pi - (A + B)^2/(4T)$
0	8.6'-1	2.3'-1
1	4.6'-2	1.0'-3
2	8.8'-5	7.4'-9
3	3.1'-10	1.8'-19
4	3.7'-21	5.5'-41
5	5.5'-43	2.4'-84
6	1.2'-86	2.3'-171
7	5.8'-174	1.1'-345
8	1.3'-348	1.1'-694
9	6.9'-698	6.1'-1393

Since the A-G mean iteration converges with order 2, we need $\sim \log_2 n$ iterations to obtain precision n. Each iteration involves one (precision n) square root, one multiplication, one squaring, one multiplication by a power of two, and some additions. Thus, from the results of Section 2, the time required to evaluate π is $\sim \frac{15}{2} M(n) \log_2 n$.

Comments

1. Unlike Newton's iteration, the A-G mean iteration is not self-correcting. Thus, we cannot start with low precision

and increase it, as was possible in Section 2.

2. Since there are $\sim\log_2 n$ iterations, we may lose $O(\log\log(n))$ bits of accuracy through accumulation of rounding errors, even though the algorithm is numerically stable. Thus, it may be necessary to work with precision $n + O(\log\log(n))$. From (1.3), the time required is still $\sim\frac{15}{2}M(n)\log_2 n$.

9. MULTIPLE-PRECISION EVALUATION OF LOG(X)

There are several algorithms for evaluating $\log(x)$ to precision n in time $O(M(n)\log(n))$. For example, a method based on Landen transformations of incomplete elliptic integrals is described in Brent [75b]. The method described here is essentially due to Salamin (see Beeler et al [72]), though the basic relation (9.1) was known by Gauss.

If $\cos(\phi) = \varepsilon^{\frac{1}{2}}$ is small, then

$$K(\phi) = (1 + O(\varepsilon))\log(4\varepsilon^{-\frac{1}{2}}) \tag{9.1}$$

Thus, taking $a_0 = 1$, $b_0 = 4/y$, where $y = 4\varepsilon^{-\frac{1}{2}}$, and applying the A-G mean iteration to compute $a = \lim_{i\to\infty} a_i$, gives

$$\log(y) = \frac{\pi}{2a}\,(1 + O(y^{-2}))$$

for large y. Thus, so long as $y \geq 2^{n/2}$, we can evaluate $\log(y)$ to precision n. If $\log(y) = O(n)$ then $\sim 2\log_2 n$ iterations are required, so the time is $\sim 13M(n)\log_2 n$, assuming π is precomputed.

For example, to find $\log(10^6)$ we start the A-G mean iteration with $a_0 = 1$ and $b_0 = 4'\text{-}6$. Results of the first seven iterations are given to 10 significant figures in Table 9.1. We find that $\pi/(2a_7) = 13.81551056$, which is correct.

Table 9.1: Computation of $\log(10^6)$

i	a_i	b_i
0	1.000000000'0	4.000000000'-6
1	5.000020000'-1	2.000000000'-3
2	2.510010000'-1	3.162283985'-2
3	1.413119199'-1	8.909188753'-2
4	1.152019037'-1	1.122040359'-1
5	1.137029698'-1	1.136930893'-1
6	1.136980295'-1	1.136980294'-1
7	1.136980295'-1	1.136980295'-1

Since $\log(2) = \frac{1}{n}\log(2^n)$, we can evaluate $\log(2)$ to precision n in time $\sim 13M(n)\log_2 n$. Suppose $x \in [b,c]$, where $b > 1$. We may set $y = 2^n x$, evaluate $\log(y)$ as above, and use the identity

$$\log(x) = \log(y) - n.\log(2)$$

to evaluate $\log(x)$. Since $\log(y) \simeq n.\log(2)$, approximately $\log_2 n$ significant bits will be lost through cancellation, so it is necessary to work with precision $n + O(\log(n))$.

If x is very close to 1 , we have to be careful in order to obtain $\log(x)$ with a small relative error. Suppose $x = 1 + \delta$. If $|\delta| < 2^{-n/\log(n)}$ we may use the power series

$$\log(1 + \delta) = \delta - \delta^2/2 + \delta^3/3 - \ldots ,$$

and it is sufficient to take about $\log(n)$ terms. If δ is larger, we may use the above A-G mean method, with working precision $n + O(n/\log(n))$ to compensate for any cancellation.

Finally, if $0 < x < 1$, we may use $\log(x) = -\log(1/x)$, where $\log(1/x)$ is computed as above. To summarize, we have proved:

Theorem 9.1

If $x > 0$ is a precision n number, then $\log(x)$ may be evaluated to precision n in time $\sim 13M(n)\log_2 n$ as $n \to \infty$ [assuming π and $\log(2)$ precomputed to precision $n + O(n/\log(n))$].

Note: The time required to compute $\log(x)$ by the obvious power series method is $O(nM(n))$. Since $13\log_2 n < n$ for $n \geq 83$, the method described here may be useful for moderate n, even if the classical $O(n^2)$ multiplication algorithm is used.

10. MULTIPLE-PRECISION EVALUATION OF EXP(X)

Corresponding to Theorem 9.1, we have:

Theorem 10.1

If $[a,b]$ is a fixed interval, and $x \in [a,b]$ is a precision n number such that $\exp(x)$ does not underflow or overflow, then $\exp(x)$ can be evaluated to precision n in time $\sim 13M(n)\log_2 n$ as $n \to \infty$ (assuming π and $\log(2)$ are precomputed).

Proof

To evaluate $\exp(x)$ we need to solve the equation $f(y) = 0$, where $f(y) = \log(y) - x$, and x is regarded as constant. Since

$$f^{(k)}(y) = (-1)^{k-1}\,(k-1)!\,y^{-k}$$

can be evaluated in time $O(M(n)) = o(M(n)\log(n))$ for any fixed $k \geq 1$, the result follows from Theorems 6.1 and 9.1. [The $(k+1)$-th order method in the proof of Theorem 6.1 may simply be taken as

$$y_{i+1} = y_i \sum_{j=0}^{k} (x - \log(y_i))^j/j!\ ]$$

11. MULTIPLE-PRECISION OPERATIONS ON COMPLEX NUMBERS

Before considering the multiple-precision evaluation of trigonometric functions, we need to state some results on multiple-precision operations with complex numbers. We assume that a precision n complex number $z = x + iy$ is represented as a pair (x, y) of precision n real numbers. As before, a precision n operation is one which gives a result with a relative error $O(2^{-n})$. (Now, of course, the relative error may be complex, but its absolute value must be $O(2^{-n})$.) Note that the smaller component of a complex result may occasionally have a large relative error, or even the wrong sign!

Complex Multiplication

Since $z = (t + iu)(v + iw) = (tv - uw) + i(tw + uv)$, a complex multiplication may be done with four real multiplications and two additions. However, we may use an idea of Karatsuba and Ofman [62] to reduce the work required to three real multiplications and some additions: evaluate tv, uw, and $(t + u)(v + w)$, then use

$$tw + uv = (t + u)(v + w) - (tv + uw) .$$

Since $|t + u| \leq 2^{\frac{1}{2}}|t + iu|$ and $|v + w| \leq 2^{\frac{1}{2}}|v + iw|$, we have

$$|(t + u)(v + w)| \leq 2|z| .$$

Thus, all rounding errors are of order $2^{-n}|z|$ or less, and the computed product has a relative error $O(2^{-n})$. The time for the six additions is asymptotically negligible compared to that for the three multiplications, so precision n complex multiplication may be performed in time $\sim 3M(n)$.

Complex Squares

Since $(v + iw)^2 = (v - w)(v + w) + 2ivw$, a complex

square may be evaluated with two real multiplications and additions, in time $\sim 2M(n)$.

Complex Division

Using complex multiplication as above, and the same division algorithm as in the real case, we can perform complex division in time $\sim 12M(n)$. However, it is faster to use the identity

$$\frac{t + iu}{v + iw} = (v^2 + w^2)^{-1}[(t + iu)(v - iw)] ,$$

reducing the problem to one complex multiplication, four real multiplications, one real reciprocal, and some additions. This gives time $\sim 10M(n)$. For complex reciprocals we have $t = 1$, $u = 0$, and time $\sim 7M(n)$.

Complex Square Roots

Using (2.2) requires, at the last iteration, one precision n complex squaring and one precision n/2 complex division. Thus, the time required is $\sim 2(2 + 10/2)M(n) = 14M(n)$.

Complex A-G Mean Iteration

From the above results, a complex square root and multiplication may be performed in time $\sim 17M(n)$. Each iteration transforms two points in the complex plane into two new points, and has an interesting geometric interpretation.

12. MULTIPLE-PRECISION EVALUATION OF TRIGONOMETRIC FUNCTIONS

Since

$$\log(v + iw) = \log|v + iw| + i.\arctan(w/v) \tag{12.1}$$

and

$$\exp(i\theta) = \cos(\theta) + i.\sin(\theta) , \tag{12.2}$$

we can evaluate $\arctan(x)$, $\cos(x)$ and $\sin(x)$ if we can evaluate $\log(z)$ and $\exp(z)$ for complex arguments z . This

may be done just as described above for real z, provided we choose the correct value of $(a_j b_j)^{\frac{1}{2}}$. Some care is necessary to avoid excessive cancellation; for example, we should use the power series for $\sin(x)$ if $|x|$ is very small, as described above for $\log(1 + \delta)$. Since $\sim 2\log_2 n$ A-G mean iterations are required to evaluate $\log(z)$, and each iteration requires time $\sim 17M(n)$, we can evaluate $\log(z)$ in time $\sim 34M(n)\log_2 n$. From the complex version of Theorem 6.1, $\exp(z)$ may also be evaluated in time $\sim 34M(n)\log_2 n$.

As an example, consider the evaluation of $\log(z)$ for $z = 10^6(2 + i)$. The A-G mean iteration is started with $a_0 = 1$ and $b_0 = 4/z = 1.6'\text{-}6 - (8.0'\text{-}7)i$. The results of six iterations are given, to 8 significant figures, in Table 12.1.

Table 12.1: Evaluation of $\log 10^6(2 + i)$.

j	a_j	b_j
0	(1.0000000'0, 0.0000000'0)	(1.6000000'-6, -8.0000000'-7)
1	(5.0000080'-1, -4.0000000'-7)	(1.3017017'-3, -3.0729008'-4)
2	(2.5065125'-1, -1.5384504'-4)	(2.5686505'-2, -2.9907884'-3)
3	(1.3816888'-1, -1.5723167'-3)	(8.0373334'-2, -4.6881008'-3)
4	(1.0927111'-1, -3.1302088'-3)	(1.0540970'-1, -3.6719673'-3)
5	(1.0734040'-1, -3.4010880'-3)	(1.0732355'-1, -3.4064951'-3)
6	(1.0733198'-1, -3.4037916'-3)	(1.0733198'-1, -3.4037918'-3)

We find that $\frac{\pi}{2a_7} = 14.620230 + 0.46364761i$

$\simeq \log|z| + i.\arctan(\frac{1}{2})$

as expected.

Another method for evaluating trigonometric functions in time $O(M(n)\log(n))$, without using the identities (12.1) and (12.2), is described in Brent [75b].

13. OPERATIONS ON FORMAL POWER SERIES

There is an obvious similarity between a multiple-precision number with base β_i :

$$\beta^e \sum_{i=1}^{n} a_i \beta^{-i} \quad (0 \leq a_i < \beta) ,$$

and a formal power series:

$$\sum_{i=0}^{\infty} a_i x^i \qquad (a_i \text{ real, } x \text{ an indeterminate}) .$$

Thus, it is not surprising that algorithms similar to those described in Section 2 may be used to perform operations on power series.

In this section only, $M(n)$ denotes the number of scalar operations required to evaluate the first n coefficients $c_0,\ldots,c_{n-1}$ in the formal product

$$\left(\sum_{i=0}^{\infty} a_i x^i\right)\left(\sum_{i=0}^{\infty} b_i x^i\right) = \sum_{i=0}^{\infty} c_i x^i .$$

Clearly, c_j depends only on $a_0,\ldots,a_j$ and $b_0,\ldots,b_j$, in fact

$$c_j = \sum_{i=0}^{j} a_i b_{j-i} .$$

The classical algorithm gives $M(n) = O(n^2)$, but it is possible to use the fast Fourier transform (FFT) to obtain

$$M(n) = O(n.\log(n)) .$$

(see Borodin [73]).

If we assume that $M(n)$ satisfies conditions (1.2) and

(1.3), then the time bounds given in Section 2 for division, square roots, etc. of multiple-precision numbers also apply for the corresponding operations on power series (where we want the first n terms in the result). For example, if $P(x) = \sum_{i=0}^{\infty} a_i x^i$ and $a_0 \neq 0$, then the first n terms in the expansion of $1/P(x)$ may be found with $\sim 3M(n)$ operations as $n \to \infty$. However, some operations, e.g. computing exponentials, are much easier for power series than for multiple-precision numbers!

Evaluation of $\log(P(x))$

If $a_0 > 0$ we may want to compute the first n terms in the power series $Q(x) = \log(P(x))$. Since $Q(x) = \log(a_0) + \log(P(x)/a_0)$, there is no loss of generality in assuming that $a_0 = 1$. Suppose $Q(x) = \sum_{i=0}^{\infty} b_i x^i$. From the relation

$$Q'(x) = P'(x)/P(x) , \tag{13.1}$$

where the prime denotes formal differentiation with respect to x, we have

$$\sum_{i=1}^{\infty} i b_i x^{i-1} = \left(\sum_{i=1}^{\infty} i a_i x^{i-1} \right) \Big/ \left(\sum_{i=0}^{\infty} a_i x^i \right) . \tag{13.2}$$

The first n terms in the power series for the right side of (13.2) may be evaluated with $\sim 4M(n)$ operations, and then we need only compare coefficients to find $b_1, \ldots, b_{n-1}$. (Since $a_0 = 1$, we know that $b_0 = 0$.) Thus, the first n terms in $\log(P(x))$ may be found in $\sim 4M(n)$ operations. It is interesting to compare this result with Theorem 9.1.

Evaluation of $\exp(P(x))$

If $R(x) = \exp(P(x))$ then $R(x) = \exp(a_0)\exp(P(x) - a_0)$, so there is no loss of generality in assuming that $a_0 = 0$. Now $\log(R(x)) - P(x) = 0$, and we may regard this as an

equation for the unknown power series $R(x)$, and solve it by one of the usual iterative methods. For example, Newton's method gives the iteration

$$(13.3)\quad R_{i+1}(x) = R_i(x) - R_i(x)(\log(R_i(x)) - P(x)) .$$

If we use the starting approximation $R_0(x) = 1$, then the terms in $R_k(x)$ agree exactly with those in $R(x)$ up to (but excluding) the term $O(x^{2^k})$. Thus, using (13.3), we can find the first n terms of $\exp(P(x))$ in $\sim 9M(n)$ operations, and it is possible to reduce this to $\sim\frac{22}{3}M(n)$ operations by using a fourth-order method instead of (13.3). Compare Theorem 10.1.

Evaluation of P^m

Suppose we want to evaluate $(P(x))^m$ for some large positive integer m. We can assume that $a_0 \neq 0$, for otherwise some power of x may be factored out. Also, since $P^m = a_0^m(P/a_0)^m$, we can assume that $a_0 = 1$. By forming P^2, P^4, P^8, ..., and then the appropriate product given by the binary expansion of m, we can find the first n terms of P^m in $O(M(n)\log_2 m)$ operations. Surprisingly, this is <u>not</u> the best possible result, at least for large m. From the identity

$$(13.4)\qquad P^m = \exp(m.\log(P))$$

and the above results, we can find the first n terms of P^m in $O(M(n))$ operations! (If $a_0 \neq 1$, we also need $O(\log_2 m)$ operations to evaluate a_0^m.) If the methods described above are used to compute the exponential and logarithm in (13.4), then the number of operations is $\sim\frac{34}{3}M(n)$ as $n \to \infty$.

Other Operations on Power Series

The method used to evaluate $\log(P(x))$ can easily be generalized to give a method for $f(P(x))$, where $df(t)/dt$

is a function of t which may be written in terms of square roots, reciprocals etc. For example, with $f(t) = \arctan(t)$ we have $df/dt = 1/(1 + t^2)$, so it is easy to evaluate $\arctan(P(x))$. Using Newton's method we can evaluate the inverse function $f^{(-1)}(P(x))$ if $f(P(x))$ can be evaluated. Generalizations and applications are given in Brent and Kung [75].

Some operations on formal power series do not correspond to natural operations on multiple-precision numbers. One example, already mentioned above, is formal differentiation. Other interesting examples are composition and reversion. The classical composition and reversion algorithms, as given in Knuth [69], are $O(n^3)$, but much faster algorithms exist: see Brent and Kung [75].

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) We consider methods for finding high-precision approximations to simple zeros of smooth functions. As an application, we give fast methods for evaluating the elementary functions log(x), exp(x), sin(x) etc. to high precision. For example, if x is a positive floating-point number with an n-bit fraction, then (under rather weak assumptions) an n-bit approximation to log(x) or exp(x) may be computed in time asymptotically equal to $13M(n)\log_2 n$ as $n \to \infty$, where M(n) is the time required to multiply floating-point numbers with n-bit fractions. Similar results are given for the other elementary functions, and some analogies with operations on formal power series are mentioned.

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