

Validated Bounds for Taylor Coefficients of Analytic Functions

MARKUS NEHER

*Institut für Angewandte Mathematik, Universität Karlsruhe, D-76128 Karlsruhe, Germany,
e-mail: markus.neher@math.uni-karlsruhe.de*

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Abstract. We present methods for the practical computation of verified bounds for Taylor coefficients of analytic functions. The bounds are constructed from Cauchy's estimate and from some of its modifications. Interval arithmetic is used to obtain rigorous results.

1. Introduction

The intention of this paper originates from the general Taylor series method: Let

$$f(z) = \sum_{j=0}^{\infty} a_j z^j, \quad |z| \leq r,$$

be a given analytic function in a disc with radius $r > 0$, centered at the origin of the complex plane, let (f_1, \dots, f_n) , $n \in \mathbb{N}$, denote a vector of n functions with the above properties and let F be an abstract operator such that the equation

$$F(y; f_1, \dots, f_n) = 0 \tag{1.1}$$

uniquely defines an analytic function $y(z) = \sum_{j=0}^{\infty} b_j z^j$ with (arbitrary) positive radius of convergence. The Taylor series method for the solution of (1.1) then aims at determining the unknown coefficients b_j via recurrence relations that are obtained by inserting the respective series representations of f_1, \dots, f_n into (1.1), equating the terms with equal powers and solving the numbers b_j . Only a finite number of the coefficients b_j can be calculated in practical computations. In this case, a finite sum

$$\tilde{y}(z) = \sum_{j=0}^{\kappa-1} b_j z^j$$

only yields an approximation to $y(z)$, where the approximation error $y(z) - \tilde{y}(z)$ given by the infinite series

$$t(z) := \sum_{j=\kappa}^{\infty} b_j z^j \quad (1.2)$$

can generally not be explicitly calculated. On the other hand, a computable bound for the approximation error would be sufficient to obtain a validated solution of (1.1). E.g., if a geometric series bound for t was known, that is if an estimate for the unknown coefficients in (1.2) of the form

$$|b_j| \leq \frac{M}{r^j} \quad \text{for } j \geq \kappa \quad (1.3)$$

was available, then the remainder series t could be bounded by

$$|t(z)| \leq M \sum_{j=\kappa}^{\infty} \left(\frac{z}{r}\right)^j = \frac{M \left(\frac{z}{r}\right)^{\kappa}}{1 - \frac{z}{r}} \quad \text{for } |z| < r.$$

Indeed, the estimate (1.3) can be derived from geometric series bounds for the Taylor coefficients of f_1, \dots, f_n . We illustrate this with the following example: Consider the initial value problem

$$\begin{cases} y' - y^2 - f(x) = 0, & x > 0 \\ y(0) - \eta = 0, \end{cases} \quad (1.4)$$

where $f(x) = \sum_j a_j x^j$, $|x| \leq r$, is a given function. Inserting the series expansion of f and a presumable series expansion $y = \sum_j b_j x^j$ into (1.4), we get

$$b_0 = \eta, \quad b_{j+1} = \frac{1}{j+1} \sum_{v=0}^j b_v b_{j-v} + a_j, \quad j \in \mathbb{N}_0, \quad (1.5)$$

which yields a power series solution of (1.4) if the radius of convergence of $\sum_j b_j x^j$ can be proved to be positive.

Now suppose that there is some $A > \eta^2$ such that $|a_j r^j| \leq A$ holds for all $j \geq 0$ and let

$$\tilde{r} := \min \left\{ \frac{1}{2\sqrt{A}}, r \right\}. \quad (1.6)$$

By induction, we will prove that $|b_j \tilde{r}^j| \leq \sqrt{A}$ holds for all $j \geq 0$: From (1.5), we have $|b_0 \tilde{r}^0| = |b_0| = |\eta| \leq \sqrt{A}$. Assuming that $|b_\nu \tilde{r}^\nu| \leq \sqrt{A}$ holds for $\nu = 0, 1, \dots, j$, we get from (1.5)

$$\begin{aligned} |b_{j+1} \tilde{r}^{j+1}| &= \tilde{r} \left| \frac{1}{j+1} \sum_{\nu=0}^j b_\nu \tilde{r}^\nu b_{j-\nu} \tilde{r}^{j-\nu} + a_j \tilde{r}^j \right| \\ &\leq \tilde{r} \left(\frac{1}{j+1} \sum_{\nu=0}^j A + A \frac{\tilde{r}^j}{r^j} \right) = \tilde{r} A \left(1 + \left(\frac{\tilde{r}}{r} \right)^j \right) \leq \sqrt{A}, \end{aligned}$$

where the last inequality follows from (1.6). Hence, the series $\sum_j b_j x^j$ converges for $x \in [0, \tilde{r})$ and we have

$$\left| y(x) - \sum_{j=0}^{\kappa-1} b_j x^j \right| \leq \sqrt{A} \frac{\left(\frac{x}{\tilde{r}} \right)^\kappa}{1 - \frac{x}{\tilde{r}}}.$$

The right hand side of the last inequality is a computable bound of the approximation error that becomes arbitrarily small for a sufficiently large κ .

In [10]–[12], the above stated error analysis for the Taylor series method was applied to the solution of initial value problems for linear and nonlinear ODEs. It is generally applicable if equations can be derived from (1.1) such that the series bounds for f_1, \dots, f_n give rise to a computable series bound for t .

We will not pursue the general Taylor series method and its error estimation any further in this paper. Instead we study its prerequisite, that is the computation of bounds for the Taylor coefficients of explicitly known analytic functions. The functions considered are those that are usually available on a computer: rational functions, the function $\exp(z)$, compositions like $\exp(z^2)$ or $\sin(z) = \frac{\exp(iz) - \exp(-iz)}{2i}$, and branches of inverse functions like $\text{Log}(z)$. For the Taylor remainder series of these functions we will provide computable bounds in the form of geometric series or in the form of derivatives of geometric series.

An important tool for our calculations will be interval arithmetic. We assume that the reader is familiar with interval computations as described in [1], [9], [13]. Throughout this paper, a complex interval Z is defined by a pair of two real intervals $X = [\underline{x}, \bar{x}]$ and $Y = [\underline{y}, \bar{y}]$ in the following way:

$$Z = X + iY := \{z = x + iy : x \in X, y \in Y\},$$

where $i^2 = -1$.

Our analysis could also be formulated in circular complex arithmetic [6], [14]. We did not use circular complex intervals, however, due to software limitations. Our software implementation of the methods of this paper relied on a library of complex functions that had been written in rectangular complex interval arithmetic.

The paper is structured as follows: In the next section, we describe the rigorous computation of Cauchy's estimate on the computer. Following this, we propose three alternatives to Cauchy's estimate and we discuss their respective advantages with regard to accuracy and its suitability in practical calculations. In the final section, numerical examples are given.

2. Cauchy's Estimate on the Computer

In the following, let $r > 0$, let B be the disc $\{z : |z| < r\}$, and let C be the circle $\{z : |z| = r\}$.

A well known bound for the Taylor coefficients of an analytic function is Cauchy's estimate (cf. [5, p. 84]): a function $f(z)$ that is analytic in B and bounded on C has a power series expansion

$$f(z) = \sum_{j=0}^{\infty} a_j z^j, \quad |z| \leq r,$$

for which

$$|a_j| \leq \frac{M(r)}{r^j}, \quad j \in \mathbb{N}_0, \quad (2.1)$$

holds, where

$$M(r) := \max_{|z|=r} |f(z)|.$$

The inequality (2.1) is known as Cauchy's estimate.

At first glance it might seem obvious to calculate $M(r)$ in the following way: A parametric representation of C , i.e. $z = re^{it}$, $t \in [0, 2\pi]$, is used to split $f(z)$ into $f(z) = u(t) + iv(t)$ with real-valued functions u and v . $M(r)$ is then the maximum value of the real-valued function $\sqrt{u^2 + v^2}$ on $[0, 2\pi]$, a well-understood one-dimensional problem. However, the computation of $\sqrt{u^2 + v^2}$ requires lengthy manual calculations or calculations by some computer algebra system, furthermore its automation for arbitrary functions appears difficult.

Hence, we rather cover C equiangularly with a number of complex intervals Z_k , $k = 1, \dots, k_{\max}$. Using appropriate interval functions, for each k an interval $[E_k, \overline{F}_k]$

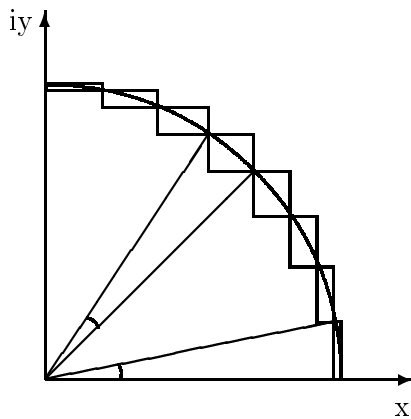


Figure 1. Equiangular interval covering.

that encloses $|f(Z_k)|$ (the range of $|f|$ on Z_k) is computed, and an upper bound for $M(r)$ is then obtained from the maximum value of the numbers \overline{F}_k .

This approach is better suited for automatic computation, even though the covering of C by two-dimensional intervals leads to an overestimation of $M(r)$. If $f(z)$ is a composition of rational functions or complex standard functions (including branches of inverse trigonometric or inverse hyperbolic functions) then its real and imaginary parts can be expressed by compositions of real standard functions. Such decompositions have been utilized in [2], [3], [8] for the construction of complex interval standard functions that are easily implemented in modern programming languages (see also [16] for a detailed description of various computer methods for the range of functions).

An accurate upper bound for $M(r)$ can only be expected for sufficiently small diameters of the covering intervals Z_k for an arbitrary function. For this, we employ one of the global optimization methods from [17]. The intervals Z_k of some initial covering of C are gathered in a list L . For each element of L , an absolute function value enclosure $[\underline{f}_k, \overline{f}_k] \ni |f(c_k)|$ at a particular point $c_k \in Z_k$ and a range enclosure $[\underline{F}_k, \overline{F}_k] \supseteq |f(Z_k)|$ are computed. Now let

$$\underline{m} := \max_k \underline{f}_k.$$

Then all Z_k for which $\overline{F}_k < \underline{m}$ holds cannot contain the maximum value of $|f|$. These intervals are deleted from the list, and the remaining elements are split into subintervals, which form a new list L . This branch and bound process is continued until $M(r)$ is determined with the desired accuracy.

Even the accurate computation of $M(r)$ does not always imply good upper bounds for the Taylor coefficients of f , because Cauchy's estimate can unfortunately be

very pessimistic. E.g., for the exponential function and $r = 1$, Cauchy's estimate gives $M(1) = e$, leading to the estimation

$$\frac{1}{j!} \leq e \quad \text{for all } j \in \mathbb{N}_0,$$

which becomes more and more unsatisfactory for large j .

On the other hand, Cauchy's estimate is sharp, since equality is reached in (2.1) for the monomial $f_n(z) = z^n$ and $j = n$. To compute better bounds for the Taylor coefficients, additional information on f is required. In the next two sections, we show how information on derivatives of f can be utilized to improve Cauchy's estimate.

3. Estimates from Polynomial Approximation

THEOREM 3.1. *Let*

$$f(z) = \sum_{j=0}^{\infty} a_j z^j, \quad |z| \leq r, \quad r > 0,$$

be analytic in $B = \{z : |z| < r\}$ and bounded on $C = \{z : |z| = r\}$. Further let $p_l(z)$ denote a polynomial of order l , and let

$$g(z) := f(z) - p_l(z).$$

Then

$$|a_j| \leq \frac{N(r, l)}{r^j} \quad \text{for } j > l, \tag{3.1}$$

where

$$N(r, l) := \max_{|z|=r} |g(z)|. \tag{3.2}$$

Proof. By construction, $g(z)$ is analytic in B and bounded on C . Hence, Cauchy's estimate applies to g . The assertion then follows from the fact that the Taylor coefficients with index greater than l of f and g are the same. \square

Any polynomial p_l can theoretically be subtracted from f for the computation of $N(r, l)$, but there are several reasons why we recommend the use of the Taylor polynomial T_l in practical calculations. As was mentioned in the introduction, the

Table 1. $N(r, l) = \max_{|z|=r} |e^z - T_l(z)|$

r	l	$N(r, l)$	r	l	$N(r, l)$	r	l	$N(r, l)$
1	0	2.72E+00	10	0	2.21E+04	20	0	4.86E+08
1	5	1.62E-03	10	10	9.19E+03	20	25	5.45E+07
1	8	3.06E-06	10	20	3.50E+01	20	40	1.24E+04
1	10	2.74E-08	10	25	3.90E-01	20	50	2.35E+00
1	20	2.06E-20	10	30	1.76E-03	20	100	3.35E-29

low order Taylor coefficients of f are already required in the computation of an approximate solution \tilde{y} of the problem $F(y; f) = 0$, so that the construction of the Taylor polynomial does not require additional calculations here.

It is also an advantage that T_l can be computed easily, with the technique of automatic differentiation. Moore [9, Chapter 11] has presented algorithms for the recursive computation of Taylor coefficients for standard functions. A detailed analysis of automatic differentiation has been given in [15].

Finally, the Taylor polynomial is a *near-best* approximation of f in the maximum norm [4], so that one should not expect essentially better results employing other approximation polynomials like interpolation polynomials. Therefore, we always write T_l instead of p_l in the following, although the following considerations also apply for arbitrary polynomials.

In Table 1, we show the improvement of $N(r, l)$ with increasing l for $f(z) = e^z$ and the Taylor polynomial T_l . We have

$$N(r, l) = \max_{|z|=r} |e^z - T_l(z)| = e^r - T_l(r). \tag{3.3}$$

The numbers presented in Table 1 were computed from (3.3) with the Maple V computer algebra system.

If the computation of a guaranteed bound for $N(r, l)$ is performed in interval arithmetic, a new problem arises. The calculation of $f(Z_k) - T_l(Z_k)$ requires separate range enclosures of f and of T_l , which affects the relation between the number k_{\max} of intervals in the covering of C and the order l of the Taylor polynomial T_l . If the widths

$$w(Z_k) := \max\{|\bar{x}_k - \underline{x}_k|, |\bar{y}_k - \underline{y}_k|\}$$

of the intervals Z_k are so large that

$$\min_k |w(f(Z_k) - T_l(Z_k))| > \|f - T_l\|_\infty, \tag{3.4}$$

then no element Z_k can be deleted from the accompanying list L . Hence, the better the approximation of f by T_l , the finer must be the covering of C (i.e. the more bisections are performed in the branch and bound algorithm) for an accurate computation of a bound for $N(r, l)$.

4. Estimates from Derivatives

THEOREM 4.1. *Let*

$$f(z) = \sum_{j=0}^{\infty} a_j z^j, \quad |z| \leq r, \quad r > 0,$$

be analytic in $B = \{z : |z| < r\}$, and let the m -th derivative of f be bounded on $C = \{z : |z| = r\}$. Further, let

$$P(j, m) := (j+1) \dots (j+m), \quad P(j, 0) := 1 \quad \text{for } m \in \mathbb{N}, j \in \mathbb{N}_0.$$

Then

$$|a_j| \leq \frac{U(r, m)r^m}{P(j-m, m)r^j} \quad \text{for } j \geq m, \quad (4.1)$$

where

$$U(r, m) := \max_{|z|=r} |f^{(m)}(z)|.$$

Proof. Under the assumptions of the theorem, Cauchy's estimate applies to

$$f^{(m)}(z) = \sum_{j=0}^{\infty} P(j, m)a_{j+m}z^j,$$

which yields

$$|P(j, m)a_{j+m}| \leq \frac{U(r, m)}{r^j}. \quad \square$$

The estimate (4.1) is a considerable improvement to Cauchy's estimate. By (4.1), the remainder series of f , that is the series

$$f(z) - T_m(z) = \sum_{j=m}^{\infty} a_j z^j,$$

is bounded by a series that converges faster than a geometric series, for all $z \in B$. Note also that for $r > 1$, the bounds for $|a_j|$ improve with increasing m , for $j \rightarrow \infty$.

Comparing (4.1) with (3.1), the main advantage for practical calculations lies in the fact that there is no inherent cancellation in the interval computation of $U(r, m)$, in contrast to the interval computation of $N(r, l)$.

The last two methods can be combined for further improvement. Let S_l be the Taylor polynomial of order l for the m -th derivative of f . Then instead of (4.1), we have

$$|a_j| \leq \frac{V(r, m, l)r^m}{P(j - m, m)r^j} \quad \text{for } j > m + l, \quad (4.2)$$

where

$$V(r, m, l) := \max_{|z|=r} |f^{(m)}(z) - S_l(z)|.$$

Compared to estimate (4.1) for $m = \mu + \nu + 1$, estimate (4.2) for $m = \mu$, $l = \nu$ can be favorable in practical calculations, if the computation of high-order derivatives of f is expensive. To calculate $V(r, \mu, \nu)$, derivatives of order higher than μ must only be computed once, at $z = 0$, whereas for the calculation of $U(r, \mu + \nu + 1)$, the derivatives of order up to $\mu + \nu + 1$ are required for all Z_k .

5. Numerical Examples

The various methods proposed in this paper have been implemented in a computer program written in C-XSC [7], a C++ class library for extended scientific computing. All roundoff errors were enclosed by the C-XSC machine interval arithmetic in the result of any computation to ensure validated results. The complete code of the computer program is available via Internet at <http://www.uni-karlsruhe.de/~Markus.Neher/acetaf.html>.

Except for trivial examples it is obviously impossible to compute $M(r)$, $N(r, l)$, or $U(r, m)$ exactly. Only *validated bounds* for these constants can be calculated. Because we do not want to repeat the word “bound” again and again, we loosely speak of the computation of the constants themselves in the following.

For all examples, we show a table of $M(r)$, $N(r, l)$, and $U(r, m)$ for several radii, the resulting bounds for some of the Taylor coefficients of the respective functions, and the computation times (in seconds) that were obtained on a PC with a Pentium II processor with 333 MHz. The values of $V(r, m, l)$ were computed as well, but we omit the results of these calculations, as the improvement (compared to $U(r, m)$) was cost-effective rather than significant.

For $N(r, l)$, the order l of the Taylor polynomial was determined by the following heuristics: Following the argumentation in Section 3, for a fixed covering of C and interval extensions \mathcal{F} of f and \mathcal{T}_l of T_l , each computable upper bound for $N(r, l)$ is bounded from below by $\max_k w(\mathcal{F}(Z_k)) / 2$, independently of the order l of the Taylor polynomial that is used. Now assume that \hat{l} is so large that $T_{\hat{l}}$ is a good approximation of f , and that $\mathcal{T}_l(Z_k) \approx \mathcal{T}_{\hat{l}}(Z_k)$ holds for all $l \geq \hat{l}$ and all k . Then we have

$$\max_k |\mathcal{F}(Z_k) - \mathcal{T}_l(Z_k)| \approx \omega + \|f - T_l\|_{\infty},$$

where ω is some constant that is independent of l . By construction,

$$\omega \lesssim N(r, l) \leq \max_k |\mathcal{F}(Z_k) - \mathcal{T}_l(Z_k)|.$$

Using a small set of test intervals, we get

$$\begin{aligned} \max_{k_{\text{test}}} |\mathcal{F}(Z_{k_{\text{test}}}) - \mathcal{T}_l(Z_{k_{\text{test}}})| &- \max_{k_{\text{test}}} |f(c_{k_{\text{test}}}) - T_l(c_{k_{\text{test}}})| \\ &\lesssim N(r, l) \lesssim \max_{k_{\text{test}}} |\mathcal{F}(Z_{k_{\text{test}}}) - \mathcal{T}_l(Z_{k_{\text{test}}})|. \end{aligned} \quad (5.1)$$

In our numerical examples, an equiangular covering of C with $k_{\max} = 32768$ intervals was used, and a set of 128 test intervals in (5.1). l was determined as the smallest number for which the bounds on the left and on the right in (5.1) differed by at most 1%. From this choice and for the given covering of C and the given interval extensions \mathcal{F} and \mathcal{T}_l , the best possible bound can be at most 1% lesser than the bound we computed, and our bound is about one hundred times as large as $\|f - T_l\|_{\infty}$. As we observed in many additional calculations, taking $l - 1$ or $l - 2$ instead of l did not affect $N(r, l)$ much, yet smaller values of l yielded larger bounds for $N(r, l)$.

EXAMPLE 5.1 *Bounds for the Taylor Coefficients of e^z .* Table 2 shows the performance of the various methods for the exponential function. M and U are computed very fast. As can be observed, U yields much better bounds for the Taylor coefficients of f , but this is in part due to the simplicity of the higher order derivatives.

In this example, N is smaller than M by several powers of ten, but considering the computation times, the improvement is expensive. If we compare the computed bounds with the exact values in Table 1, the factor of 100 that was mentioned above can well be observed.

EXAMPLE 5.2 *Bounds for the Taylor Coefficients of e^{z^2} .* Again, U gives much better bounds on the Taylor coefficients of f than M , but here the computation is

Table 2. Bounds for $f(z) = e^z$.

r	l	m	$M/N/U$	a_{100}	a_{1000}	Time
1	—	—	2.8E+00	2.8E+00	2.8E+00	< 1
1	8	—	4.3E-04	4.3E-04	4.3E-04	145
1	—	50	2.8E+00	9.2E-94	9.8E-150	6
10	—	—	2.7E+04	2.7E-96	2.7E-996	< 1
10	25	—	4.1E+01	4.1E-99	4.1E-999	402
10	—	50	2.7E+04	8.6E-140	9.2E-1096	9
20	—	—	5.9E+08	4.7E-122	5.5E-1293	< 1
20	40	—	1.9E+06	1.5E-124	1.7E-1295	642
20	—	50	5.9E+08	1.7E-150	2.2E-1377	11

Table 3. Bounds for $f(z) = e^{z^2}$.

r	l	m	$M/N/U$	a_{100}	a_{1000}	Time
1	—	—	3.0E+00	3.0E+00	3.0E+00	< 1
1	16	—	8.6E-04	8.6E-04	8.6E-04	253
1	—	50	4.1E+43	1.4E-50	1.5E-106	126
5	—	—	8.2E+10	1.1E-59	8.8E-689	< 1
5	62	—	7.5E+11	9.5E-59	8.1E-688	937
5	—	50	1.3E+67	4.7E-62	4.2E-747	739

more expensive. For small radius, N can be better than M , but for $r = 5$ the situation has changed, because the interval arithmetic evaluation of $|f(Z_k) - T_l(Z_k)|$ gives rise to a large overestimation of the true value.

EXAMPLE 5.3 *Bounds for the Taylor Coefficients of $\tanh(\ln(z + 11)) / 3$.* The function of this example has a singularity at $z = -11$, and the absolute values of the derivatives of f grow strongly near that point. Hence, Cauchy’s estimate gives better bounds for the Taylor coefficients a_j of f with small indexes j than does U . Only for large indexes j , U has the advantage due to the better asymptotic behaviour for $j \rightarrow \infty$.

We also computed $N(r, l)$ for several values of r and l , but N never became smaller than M . We attribute this to the overestimation that occurred with the interval arithmetic evaluation of f and T_l .

EXAMPLE 5.4 *Bounds for the Taylor Coefficients of $\frac{\cos z}{z^2 + 101}$.* Here, f has a singularity at $z = \sqrt{101}i$, and the circle with radius 10 comes very close to this point. The computation of M and U still works, but $U(10, m)$ rapidly increases with m .

Table 4. Bounds for $f(z) = \tanh(\ln(z + 11) / 3)$.

r	l	m	$M / N / U$	a_{100}	a_{1000}	Time
1	—	—	1.4E+00	1.4E+00	1.4E+00	298
1	—	50	1.5E+12	4.8E-82	5.1E-138	431
5	—	—	1.5E+00	1.9E-70	1.6E-699	297
5	—	50	7.7E+23	2.8E-105	2.5E-790	402
10	—	—	2.3E+00	2.3E-100	2.3E-1000	297
10	—	50	3.1E+77	1.1E-66	1.1E-1022	> 1000

Table 5. Bounds for $f(z) = \frac{\cos z}{z^2 + 101}$.

r	l	m	$M / N / U$	a_{100}	a_{1000}	Time
1	—	—	1.6E-02	1.6E-02	1.6E-02	< 1
1	8	—	1.6E-06	1.6E-06	1.6E-06	281
1	—	50	3.3E+18	1.1E-75	1.2E-131	49
5	—	—	1.1E+00	1.4E-70	1.2E-699	< 1
5	22	—	1.0E-03	1.3E-73	1.1E-702	482
5	—	50	1.1E+33	3.9E-96	3.5E-781	760
10	—	—	1.3E+04	1.3E-96	1.3E-996	1
10	—	10	9.7E+24	1.5E-85	1.1E-995	> 1000
10	—	30	2.4E+80	3.1E-48	3.7E-980	> 1000
10	—	50	1.1E+142	3.4E-02	3.6E-958	589

The computation times for $U(10, 10)$ and $U(10, 30)$ exceeded the limit of our timing system. $U(10, 50)$ was calculated less accurately, and thus faster.

Conclusion

We have presented several methods for the practical calculation of validated bounds for Taylor coefficients of analytic functions. These methods have been implemented on a computer, and their applicability has been demonstrated with numerical examples.

Future work will concentrate on the improvement of the calculation of N . The present implementation uses separate range enclosures of f and of the Taylor polynomial T_l . The employment of centered form evaluations of $f - T_l$ may both speed up the computation and enhance the accuracy of the computed bound for N .

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