Fast and highly accurate computation of Chebyshev expansion coefficients of analytic functions

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Abstract

Chebyshev expansion coefficients can be computed efficiently by using the FFT, and for smooth functions the resulting approximation is close to optimal, with computations that are numerically stable. Given sufficiently accurate function samples, the Chebyshev expansion coefficients can be computed to machine precision accuracy. However, the accuracy is only with respect to absolute error, and this implies that very small expansion coefficients typically have very large relative error. Upon differentiating a Chebyshev expansion, this relative error in the small coefficients is magnified and accuracy may be lost, especially after repeated differentiation. At first sight, this seems unavoidable. Yet, in this paper, we focus on an alternative computation of Chebyshev expansion coefficients using contour integrals in the complex plane. The main result is that the coefficients can be computed with machine precision relative error, rather than absolute error. This implies that even very small coefficients can be computed with full floating point accuracy, even when they are themselves much smaller than machine precision. As a result, no accuracy is lost after differentiating the expansion, and even the 100th derivative of an analytic function can be computed with near machine precision accuracy using standard floating point arithmetic. In some cases, the contour integrals can be evaluated using the FFT, making the approach both highly accurate and fast.

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1 Introduction

Among all classical orthogonal polynomials, Chebyshev polynomials play a special role in numerical analysis due to their connection with FFT algorithms and their numerical

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They allow the accurate manipulation of continuous functions using discrete function evaluations. Yet, in spite of the useful connection to the FFT on the real line, the goal of this paper is to show that an alternative computation can make Chebyshev expansions even more accurate than they already are, at least for analytic functions. In many cases, the efficiency of the FFT can be maintained. In a companion paper, we set out to illustrate that non-trivial manipulations of the Chebyshev expansion coefficients, namely their conversion to expansions in more general Jacobi polynomials, maintain this high accuracy beyond what one may have expected.

The contents of this paper have been inspired mainly by a fast method for the computation of Legendre coefficients due to Iserles and an accurate method for the computation of high-order derivatives in the complex plane due to Bornemann. Before presenting our results, we elaborate briefly on the above references and on other existing research in this area.

1.1 Fast methods for computing polynomial expansions

Several methods have been described for the fast computation of polynomial expansion coefficients. In particular, the special case of Legendre polynomials has received the most study. A popular strategy is to use the FFT, with computations based on function evaluations at the Chebyshev points. More general sets of evaluation points have been treated using Fast Multipole Methods, using a particular matrix-factorization of the problem stated as a matrix-vector product, using non-uniform FFT’s and using numerical computation of Abel transforms. All these methods exhibit computational complexity, possibly with additional logarithmic factors, for the computation of the first \( N \) coefficients. The accuracy is sometimes restricted to a chosen small value \( \epsilon \).

Methods based on function evaluations in the Chebyshev points are, at least mathematically, equivalent to an expansion in Chebyshev polynomials of the first kind. The coefficients of this expansion can then be rearranged in varying ways in order to form the Legendre expansion or other expansions. A unique feature of the fast methods for Legendre polynomials is that the evaluation points may be in the complex plane, if the function to be approximated is analytic. We will show further on that this approach is also implicitly equivalent to expanding in a set of Chebyshev polynomials (of the second kind, in this case), and then rearranging the coefficients. We will be using the same contour integrals as in these references, and a variant which leads to the computation of expansions in Chebyshev polynomials of the first kind.

1.2 Accurate computation of high-order derivatives

Computing derivatives of a function numerically is a notoriously ill-conditioned problem, especially for high-order derivatives. It was shown by Bornemann that computation of high-order derivatives through Cauchy integrals in the complex plane is, in fact, stable. To be precise, consider the power series of a function analytic at the
origin, with radius of convergence $R$,

$$f(z) = \sum_{k=0}^{\infty} t_k z^k, \quad |z| < R.$$ 

The coefficients $t_n$ can be written as a contour integral along a disc with radius $r < R$,

$$t_n = \frac{f^{(n)}(0)}{n!} = \frac{1}{2\pi i} \oint_{|z|=r} \frac{f(z)}{z^{n+1}} dz.$$  \hfill (1.1)

Such integrals can be evaluated quickly with the FFT for a range of $n$ with the parameter $z = re^{i\theta}$. However, Bornemann showed that for each $n$ an optimal value of $r$ exists, such that evaluating the contour integral is, for most analytic functions, perfectly stable. A detailed analysis is given in [4] to characterize the optimal radius, exactly or approximately, for several classes of analytic functions. Using the optimal radius $r$ for each value of $n$ precludes the use of the FFT. However, small relative error of the coefficient $t_n$ is guaranteed. As a result, for most analytic functions $t_n$ can be computed with a number of digits close to the maximal accuracy allowed by the machine precision and with values of $n$ ranging up to millions.

### 1.3 Main results and outline of this paper

We describe and analyze an efficient way to compute expansions in Chebyshev polynomials of the first or of the second kind. The computations are performed in the complex plane. We use the trapezoidal rule for the integrals

$$a_n = \frac{1}{\pi \rho^n} \int_0^{2\pi} f \left( \frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) e^{-in\theta} d\theta$$  \hfill (1.2)

and

$$b_n = \frac{1}{2\pi \rho^n} \int_0^{2\pi} f \left( \frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) (1 - (\rho e^{i\theta})^{-2}) e^{-in\theta} d\theta.$$  \hfill (1.3)

The latter integrals (for $b_n$) are those appearing in [17, (3.5)] and in [6, (3.2)]. We show in §2 that the values $a_n$ and $b_n$ correspond to coefficients of polynomial expansions using Chebyshev polynomials of the first and second kind respectively. The value of $\rho \geq 1$ is arbitrary and limited by the analyticity of $f$.

We show in §3 that the trapezoidal rule for these integrals is always stable with respect to absolute errors of the normalized values $\rho^n a_n$ and $\rho^n b_n$. Furthermore, we show that in many cases for each $n$ an optimal value $\rho^*(n)$ exists, such that the computation is stable with respect to relative errors. This implies that also very small coefficients can be computed to high accuracy. The cases depend on the properties of $f$ in the complex plane and they correspond to the cases described by Bornemann in [4] in the context of computing high-order derivatives. The integrals (1.2) and (1.3) play the role of the Cauchy integral (1.1) in [1].

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We explore two strategies for the computation of Chebyshev coefficients in the complex plane in §4. Efficiency is maximized by using the FFT along a fixed contour in §4.1, while accuracy is maximized by optimizing the contour for each coefficient in §4.2. The theory is illustrated with several numerical examples.

Next, we show that repeated differentiation of the polynomial expansions can be performed without loss of precision in §5. Finally, we illustrate that this has a beneficial effect on the accuracy of rootfinding, in particular when applying rootfinding on the derivative of a function in order to find its maxima or inflexion points, in §6. We end the paper with some concluding remarks and questions for further research in §7.

2 Chebyshev expansion coefficients

It is well known that the Chebyshev coefficients can be computed efficiently by the FFT and that this computation is numerically stable with respect to absolute errors. In the following, we will show that this strategy remains stable when performing computations along certain contours in the complex plane. For the stability with respect to relative errors, a different theory should be considered. We begin our analysis with an alternative integral expression of Chebyshev coefficients.

2.1 Chebyshev expansion of the first kind

Let \( T_n(x) \) denote the Chebyshev polynomial of the first kind of degree \( n \), as defined by

\[
T_n(\cos \theta) = \cos(n\theta), \quad n \geq 0.
\]

If a function \( f(x) \) satisfies a Dini-Lipschitz condition on the interval \([-1, 1]\) then it can be expanded uniformly in terms of \( T_n(x) \) as \([20]\) Thm. 5.7

\[
f(x) = \sum_{n=0}^{\infty} a_n T_n(x),
\]

where the prime indicates that the first term of the sum should be halved and the coefficients are given by the integrals

\[
a_n = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x)T_n(x)}{\sqrt{1-x^2}} dx, \quad n \geq 0.
\]

We are interested in integral expressions for \( a_n \) in the complex plane. Let \( \mathcal{E}_\rho \) denote the Bernstein ellipse

\[
\mathcal{E}_\rho = \left\{ z \in \mathbb{C} \mid z = \frac{1}{2}(\rho e^{i\theta} + \rho^{-1}e^{-i\theta}), \ 0 \leq \theta \leq 2\pi \right\}.
\]

We will always assume \( \rho \geq 1 \). We denote the interior of this ellipse by

\[
\mathcal{D}_\rho = \left\{ z \in \mathbb{C} \mid z = \frac{1}{2}(re^{i\theta} + r^{-1}e^{-i\theta}), \ 1 \leq r < \rho, \ 0 \leq \theta \leq 2\pi \right\}.
\]
It is well known that the Bernstein ellipses have foci $\pm 1$ and their major and minor semiaxis lengths summing to $\rho$. In the following, we will often use the notation
\[
z(u) = \frac{1}{2}(u + u^{-1}),
\]
where typically $u = \rho e^{i\theta}$ is a point on the circle with radius $\rho$ and $z(u)$ lies on the Bernstein ellipse $E_\rho$. The inverse expression (the one that satisfies $|u| > 1$) is
\[
u(z) = z + \sqrt{z^2 - 1}.
\]

The following integral expression for $a_n$ was derived by Elliott in [12, Eqn. (28)] for entire functions $f(z)$ by using Cauchy’s integral formula. Here, we shall give a simpler proof based on Laurent series expansions. We further show that the expression remains valid for functions analytic only in a neighborhood of the interval $[-1, 1]$.

**Lemma 2.1.** If $f$ is analytic inside and on the Bernstein ellipse $E_\rho$ with $\rho > 1$, then for each $n \geq 0$ we have
\[
a_n = \frac{1}{\pi \rho^n} \int_0^{2\pi} f \left( \frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) e^{-in\theta} d\theta.
\]

**Proof.** First we recall that the Chebyshev expansion is convergent in the interior of the greatest ellipse in which $f(x)$ is analytic [24, Thm. 9.1.1]. Moreover, recall the definition of the Chebyshev polynomials of the first kind in the complex plane [20, Eqn. (1.47)]
\[
T_k(z(u)) = \frac{1}{2}(u^k + u^{-k}),
\]
which implies
\[
f(z(u)) = \sum_{n=0}^{\infty} a_n T_n(z(u))
= \frac{1}{2} \sum_{n=-\infty}^{\infty} a_{|n|} u^n,
\]
where $z(u)$ is inside or on the boundary of $E_\rho$. For each $n \geq 0$, the last equality shows that the $n$-th Chebyshev coefficient of $f(x)$ corresponds exactly the $n$-th coefficient of the Laurent series expansion of $2f(z(u))$ at the origin. Therefore, we can deduce immediately that for each $n \geq 0$,
\[
a_n = \frac{1}{2\pi i} \oint_{C_\rho} 2f(z(u))u^{-n-1} du
= \frac{1}{\pi i} \oint_{C_\rho} f(z(u))u^{-n-1} du.
\]
where $C_\rho$ denotes the circle $|u| = \rho$. Substituting $u = \rho e^{i\theta}$ into the last equality yields the desired result. \qed
We make some further comments regarding (2.2) and (2.5):

- We define the normalized Chebyshev coefficient to be $\rho^n a_n$. In spite of its dependence on the parameter $\rho$, this definition is a natural one because the FFT-based algorithms presented further on yield a small absolute error of the normalized coefficients for a given value of $\rho$.

- Letting $\rho \to 1$ and using the change of variable $x = \cos \theta$, (2.5) reduces to (2.2).

- In the same limit $\rho \to 1$, we also obtain the well known expression

$$a_n = \frac{1}{\pi} \int_0^{2\pi} f(\cos \theta) e^{-in\theta} d\theta = \frac{1}{\pi} \int_0^{2\pi} f(\cos \theta) \cos(n\theta) d\theta. \quad (2.7)$$

The last expression is often the starting point for introducing fast algorithms based on the discrete cosine or Fourier transform to evaluate the Chebyshev coefficients (see, for example, [25, 13, 16, 20]).

- Integral expressions for $a_n$ in the complex plane date back at least to Bernstein [3]. They have been used, among other purposes, to estimate the decay rates of Chebyshev coefficients (see, for example, [12, 23]). To the best of our knowledge, they have not been used for computational purposes. One obvious reason is that it is not clear whether there is any advantage in evaluating (2.5) compared to evaluating (2.7), especially in view of the existence of simple, fast and stable algorithms for the latter. Furthermore, expression (2.5) requires analyticity of $f$. We will show later on that expression (2.5) can be used to give better approximations in the sense that the relative error of each Chebyshev coefficient can be minimized by choosing an optimal value of $\rho$.

- For example, (2.5) leads to the well-known bound [23 Thm. 3.8]

$$|a_n| \leq \frac{2M}{\rho^n},$$

where $M$ is the maximum absolute value of $f$ along the Bernstein ellipse $E_\rho$.

### 2.2 Chebyshev expansion of the second kind

Let $U_n(x)$ denote the Chebyshev polynomial of the second kind of degree $n$, defined by

$$U_n(\cos \theta) = \frac{\sin(n + 1)\theta}{\sin \theta}, \quad n \geq 0.$$

The Chebyshev expansion of the second kind is given by

$$f(x) = \sum_{n=0}^{\infty} b_n U_n(x), \quad (2.8)$$
where
\[ b_n = \frac{2}{\pi} \int_{-1}^{1} \sqrt{1-x^2} f(x) U_n(x) dx. \] (2.9)

**Lemma 2.2.** If \( f \) is analytic inside and on the Bernstein ellipse \( E_\rho \) with \( \rho > 1 \), then for each \( n \geq 0 \) we have
\[ b_n = \frac{1}{2\pi \rho^n} \int_{0}^{2\pi} f \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) (1 - (\rho e^{i\theta})^{-2}) e^{-i n \theta} d\theta. \] (2.10)

**Proof.** Using the definition of the Chebyshev polynomials of the second kind in the complex plane [20 Eqn. (1.51)]
\[ U_k(z(u)) = \frac{u^{k+1} - u^{-k-1}}{u - u^{-1}}, \]
we have that
\[ f(z(u)) = \sum_{n=0}^{\infty} b_n U_n(z(u)) = \sum_{n=0}^{\infty} b_n \frac{u^{n+1} - u^{-n-1}}{u - u^{-1}}. \]

Multiplying both sides of the last equality by \( 1 - u^{-2} \) gives
\[ f(z(u))(1 - u^{-2}) = \sum_{n=0}^{\infty} b_n (u^n - u^{-n-2}). \]

For each \( n \geq 0 \), the above equality shows that \( b_n \) corresponds exactly to the \( n \)-th coefficient of the Laurent series expansion of \( f(z(u))(1 - u^{-2}) \) at the origin. Therefore, we can deduce immediately that for each \( n \geq 0 \),
\[ b_n = \frac{1}{2\pi i} \oint_{C_\rho} f(z(u))(1 - u^{-2}) u^{-n-1} du. \] (2.11)

Substituting \( u = \rho e^{i\theta} \) into the last equality yields the desired result. \( \square \)

Here, too, we will make some further comments regarding (2.10):

- Similarly as before, we define the normalized Chebyshev coefficient to be \( \rho^n b_n \).
- Letting \( \rho \to 1 \) in (2.10) yields,
\[ b_n = \frac{1}{2\pi} \int_{0}^{2\pi} f(\cos \theta)(1 - e^{-2i\theta}) e^{-i n \theta} d\theta = \frac{1}{\pi} \int_{0}^{2\pi} f(\cos \theta) \sin \theta \sin(n+1) \theta d\theta = \frac{2}{\pi} \int_{-1}^{1} \sqrt{1-x^2} f(x) U_n(x) dx, \] (2.12)
which corresponds to (2.9).
Expression (2.11) can be further written as
\[
b_n = \frac{1}{2\pi i} \oint_{C_{\rho}} f(z(u))(1 - u^{-2})u^{-n-1} du
\]
\[
= \frac{1}{\pi i} \oint_{E_{\rho}} f(z(u))u(z)^{-n-1} dz(u),
\]
(2.13)

which can be used to establish the rate of decay of the coefficients \(b_n\).

From the observation of the formulas (2.5) and (2.10), it is clear that \(a_n\) and \(b_n\) are related for all \(\rho\) by
\[
b_n = \frac{a_n - a_{n+2}}{2}.
\]
(2.14)

### 3 Absolute and relative stability

From (2.5) and (2.10) we see that both kinds of Chebyshev coefficients can be expressed in terms of contour integrals with integrands that are periodic functions of \(\theta\). Thus, these coefficients can be approximated efficiently by applying the trapezoidal rule. For a more detailed and theoretical analysis of the trapezoidal rule for periodic and analytic functions, we refer the reader to [26]. In the following we shall consider stability of the computation of the Chebyshev coefficients with respect to absolute and relative errors of the normalized coefficients, respectively.

#### 3.1 Absolute stability

For the Chebyshev coefficients of the first kind, using an \(m\)-point trapezoidal rule yields
\[
a_n(m, \rho) = \frac{2}{m\rho^n} \sum_{j=0}^{m-1} f \left( \frac{1}{2}(\rho e^{2\pi ij/m} + \rho^{-1} e^{-2\pi ij/m}) \right) e^{-2\pi ijn/m}.
\]
(3.1)

Let \(P_m\) be the set of all polynomials of degree \(\leq m\) and let
\[
\|f - s\|_{D_{\rho}} := \max_{z \in D_{\rho}} |f(z) - s(z)|.
\]

Note that by the maximum modulus principle we have the equality of norms
\[
\|f - s\|_{D_{\rho}} = \|f - s\|_{\mathcal{E}_{\rho}} := \max_{z \in \mathcal{E}_{\rho}} |f(z) - s(z)|,
\]

so that from now on we simply use \(\| \cdot \|_{\mathcal{E}_{\rho}}\).

Furthermore, let
\[
s_m(z) = \sum_{k=0}^{m-1} \eta_k T_k(z)
\]

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denote the best \((m - 1)\)-th degree polynomial approximation to \(f(z)\) on and inside the ellipse \(E_\rho\), i.e.,
\[
\|f(z) - s_m(z)\|_{E_\rho} := \inf_{s \in P_{m-1}} \|f(z) - s(z)\|_{E_\rho}.
\]

In the following, we will always assume that the sampling condition \(m > n\) holds, in order to avoid aliasing of the complex exponentials in (3.1). We refer the reader to [4, §2.1] for a discussion and justification of this condition.

**Theorem 3.1.** For \(1 \leq n < m\), we have the following error estimate
\[
|a_n - a_n(m, \rho)| \leq \frac{4}{\rho^n} \|f - s_m\|_{E_\rho} + \left|\frac{\eta_{m-n}}{\rho^m}\right|,
\]
and for \(n = 0\),
\[
|a_0 - a_0(m, \rho)| \leq 4\|f - s_m\|_{E_\rho}.
\]  

**Proof.** Let \(z(\rho, \theta) = \frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\). From (2.5) and (3.1), we have
\[
a_n - a_n(m, \rho) = \frac{1}{\pi \rho^n} \int_0^{2\pi} f(z(\rho, \theta)) e^{-in\theta} d\theta - \frac{2}{m \rho^n} \sum_{j=0}^{m-1} f(z(\rho, 2\pi j/m)) e^{-2\pi ijn/m}
\]
\[
= \frac{1}{\pi \rho^n} \int_0^{2\pi} [f(z(\rho, \theta)) - s_m(z(\rho, \theta))] e^{-in\theta} d\theta
\]
\[
+ \left(\frac{1}{\pi \rho^n} \int_0^{2\pi} s_m(z(\rho, \theta)) e^{-in\theta} d\theta - \frac{2}{m \rho^n} \sum_{j=0}^{m-1} s_m(z(\rho, 2\pi j/m)) e^{-2\pi ijn/m}\right)
\]
\[
+ \frac{2}{m \rho^n} \sum_{j=0}^{m-1} [s_m(z(\rho, 2\pi j/m)) - f(z(\rho, 2\pi j/m))] e^{-2\pi ijn/m}.
\]

We use \(E_1\) to denote the first integral of the last equality, \(E_2\) denotes the difference contained in the brackets and \(E_3\) denotes the remaining part. Explicit estimates can be established for \(E_1\) and \(E_3\),
\[
|E_1| \leq \frac{2}{\rho^n} \|f - s_m\|_{E_\rho}, \quad |E_3| \leq \frac{2}{\rho^n} \|f - s_m\|_{E_\rho}.
\]

For \(E_2\), using (2.6) we have
\[
E_2 = \frac{1}{\pi \rho^n} \int_0^{2\pi} s_m(z(\rho, \theta)) e^{-in\theta} d\theta - \frac{2}{m \rho^n} \sum_{j=0}^{m-1} s_m(z(\rho, 2\pi j/m)) e^{-2\pi ijn/m}
\]
\[
= \eta_n - \frac{1}{m \rho^n} \sum_{k=-m}^{m-1} \eta_{|k|} \rho^k \left(\sum_{j=0}^{m-1} e^{2\pi ij(k-n)/m}\right)
\]
\[
= \begin{cases} 
0, & n = 0, \\
-\frac{\eta_{m-n}}{\rho^m}, & 1 \leq n < m.
\end{cases}
\]

Combining this with estimates of \(E_1\) and \(E_3\) gives the desired results. \(\square\)
From Theorem 3.1 we can see that if \( f \) is a polynomial of degree \( n \), then we have \( s_m = f \) if \( m \geq n + 1 \). This implies that the trapezoidal rule (3.1) computes the \( k \)-th Chebyshev coefficient of \( f \) exactly if \( m \geq k + n + 1 \) since \( \eta_{m-n} = 0 \). Thus, if we choose \( m \geq 2n + 1 \), then all Chebyshev coefficients of the polynomial function \( f \) can be computed exactly by the trapezoidal rule (3.1).

Theorem 3.1 implies for any function \( f \) that the difference in the normalized coefficients \( \rho^n a_n - \rho^n a_n(m, \rho) \) is on the order of \( \epsilon \), if \( m \) is sufficiently large so that \( \eta_{m-n} \) is small. This assertion is true, since from

\[
|\eta_k - a_k| = \left| \frac{1}{\pi i} \int_C (s_m(z)) f(z) e^{-n-1} du \right|
\leq \frac{2}{\rho^k} \|f(z) - s_m(z)\| \varepsilon, 
\]

it follows that

\[
|\eta_k| \leq |a_k| + \frac{2}{\rho^k} \|f(z) - s_m(z)\| \varepsilon, 
\]

\[
\leq \frac{2}{\rho^k} (M + \|f(z) - s_m(z)\| \varepsilon). 
\]

This estimate implies that the coefficients \( \eta_k \) decay exponentially fast.

Similarly, for the Chebyshev coefficients \( b_n \), the \( m \)-point trapezoidal rule gives

\[
b_n(m, \rho) = \frac{1}{m \rho^n} \sum_{j=0}^{m-1} f(z(\rho, 2\pi j/m)) (1 - \rho^{-2} e^{-4\pi ij/m}) e^{-2\pi ij/m}. 
\]

(3.4)

**Theorem 3.2.** We have the following error estimate

\[
|b_n - b_n(m, \rho)| \leq \frac{2(1 - \rho^{-2})}{\rho^2} \|f - s_m\| \varepsilon + \left\{ \begin{array}{ll}
\frac{|\eta_{m-2}|}{2 \rho^m}, & n = 0, \\
\frac{|\eta_{m-n-2} - \eta_{m-n}|}{2 \rho^m}, & n = 1, \ldots, m-3, \\
\frac{|\eta_{m-n} - \eta_{m-n+2}|}{2 \rho^m}, & n = m-2, m-1.
\end{array} \right.
\]

(3.5)

**Proof.** The proof is essentially the same as that of Theorem 3.1. We omit the details. \( \Box \)

Similarly to (3.1), if \( f \) is a polynomial of degree \( n \), then \( b_k \) is computed exactly by the trapezoidal rule (3.4) if \( m \geq k + n + 3 \). This implies that all \( \{b_k\}_{k=0}^{n} \) are computed exactly by the trapezoidal rule (3.1) if we choose \( m \geq 2n + 3 \).

Suppose now that \( \hat{f} \) is a perturbation of \( f \) and

\[
\|\hat{f}(z) - f(z)\| \varepsilon, \leq \epsilon. 
\]

The perturbed Chebyshev coefficients are given by

\[
\hat{a}_n = \frac{1}{\pi \rho^n} \int_0^{2\pi} \hat{f} \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) e^{-in\theta} d\theta. 
\]

(3.6)
Meanwhile, the computed Chebyshev coefficients are given by
\[ \hat{a}_n(m, \rho) = \frac{2}{m \rho^n} \sum_{j=0}^{m-1} \hat{f} \left( \frac{1}{2} \left( \rho e^{2\pi i j/m} + \rho^{-1} e^{-2\pi i j/m} \right) \right) e^{-2\pi i j n/m}. \] (3.7)

A simple bound can be derived for the Chebyshev coefficients of the first kind
\[ |a_n - \hat{a}_n| \leq \frac{2\epsilon}{\rho^n}, \quad |\hat{a}_n(m, \rho) - a_n(m, \rho)| \leq \frac{2\epsilon}{\rho^n}. \] (3.8)

Then the following estimate also holds
\[ \rho^n |\hat{a}_n(m, \rho) - a_n| \leq \rho^n |a_n(m, \rho) - \hat{a}_n(m, \rho)| + \rho^n |a_n - a_n(m, \rho)| \]
\[ \leq 2\epsilon + \left\{ \begin{array}{ll} 4\|f - s_m\|_{\mathcal{E}_\rho}, & n = 0, \\ 4\|f - s_m\|_{\mathcal{E}_\rho} + \left| \eta_m - n \right|_{\rho^n}, & 1 \leq n < m. \end{array} \right. \]

A similar estimate can be established for the coefficients of the second kind \( b_n \).

We conclude that the trapezoidal rule for the Chebyshev coefficients is numerically stable with respect to the absolute error of the normalized coefficients. If we only consider this absolute stability, then it is sufficient to choose the same \( \rho \) simultaneously for all Chebyshev coefficients and to compute these coefficients with the same trapezoidal rule. Furthermore, from (3.1) we see that the sum on the right hand side is perfectly suitable to utilize the FFT. Thus, the first \( N \) Chebyshev coefficients can be efficiently evaluated with a single FFT in \( \mathcal{O}(N \log N) \) operations.

### 3.2 Relative stability

If we consider the relative error of the computed coefficients, computing all Chebyshev coefficients with a single \( \rho \) is not optimal. A comprehensive analysis of the relative stability of computing the Taylor expansion coefficients of analytic functions from contour integrals along circles in the complex plane has been given by Bornemann in [4]. Here we extend his analysis to the current setting of Chebyshev coefficients.

Suppose \( \hat{f} \) is a perturbation of \( f \) with the form
\[ \hat{f}(z) = f(z)(1 + \epsilon_{\rho}(z)), \quad |\epsilon_{\rho}(z)| \leq \epsilon. \]

There is a simple upper bound on the error of the perturbed Chebyshev coefficients,
\[ |a_n - \hat{a}_n| = \frac{1}{\pi \rho^n} \left| \int_0^{2\pi} f \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) \epsilon_{\rho} \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) e^{-in\theta} d\theta \right| \]
\[ \leq \frac{\epsilon}{\pi \rho^n} \int_0^{2\pi} \left| f \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) \right| d\theta, \]
which leads to
\[ \frac{|a_n - \hat{a}_n|}{|a_n|} \leq \kappa^{Ch1}(n, \rho) \epsilon, \] (3.9)
where the quantity
\[
\kappa_{Ch1}(n, \rho) = \frac{\int_0^{2\pi} |f \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) | d\theta}{|\int_0^{2\pi} f \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) e^{-in\theta} d\theta|} \geq 1, \tag{3.10}
\]
is called the condition number of the integral. Similarly, for the Chebyshev coefficients of the second kind, we have
\[
\left| b_n - \hat{b}_n \right| \leq \kappa_{Ch2}(n, \rho) \epsilon, \tag{3.11}
\]
with the corresponding condition number given by
\[
\kappa_{Ch2}(n, \rho) = \frac{\int_0^{2\pi} |f \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) (1 - (\rho e^{i\theta})^{-2})| d\theta}{|\int_0^{2\pi} f \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) (1 - (\rho e^{i\theta})^{-2}) e^{-in\theta} d\theta|}. \tag{3.12}
\]

### 3.3 Condition number of the contour integrals

We consider the condition number of the integral expressions for the Chebyshev coefficients of the first kind. The corresponding integrals for the Chebyshev coefficients of the second kind can be analyzed similarly.

We first rewrite the condition number as
\[
\kappa_{Ch1}(n, \rho) = \frac{M(\rho)}{|a_n| \rho^n}, \tag{3.13}
\]
where
\[
M(\rho) = \frac{1}{\pi} \int_0^{2\pi} \left| f \left( \frac{1}{2} (\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right) \right| d\theta. \tag{3.14}
\]
Note that \( M(\rho) = M(\rho^{-1}) \).

We proceed by analyzing this function \( M(\rho) \). It is the analogue of the function \( M_1(r) \). It is the analogue of the function
\[
M_1(r) = \frac{1}{2\pi} \int_0^{2\pi} |f(re^{i\theta})| d\theta, \tag{3.15}
\]
which appears in the condition number for the Cauchy integral in the analysis of Bornemann. He showed that \( M_1(r) \) has a unique minimum at a finite value of \( r \). The starting point of this analysis is a theorem on the growth of \( M_1(r) \) [4, Thm 4.1] originally due to Hardy in 1915 [14]. Unfortunately, Hardy’s original proof for \( M_1(r) \) does not apply for the analysis of the function \( M(\rho) \), since the integrand of \( M(\rho) \) is not analytic at the origin. In the following theorem we formulate the corresponding result for \( M(\rho) \), with a method of proof that still largely follows that of Hardy.

**Theorem 3.3.** Let \( f \) be analytic in any ellipse \( \mathcal{E}_\rho \) with \( 1 \leq \rho < R \). The function \( M(\rho) \) satisfies the following properties:

1. \( M(\rho) \) is continuously differentiable.
2. If \( f \) is not a constant, \( M(\rho) \) is increasing as \( \rho \) grows.

3. If \( f \not\equiv 0 \), then \( \log M(\rho) \) is a convex function of \( \log \rho \).

**Proof.** Let \( g(z) = f(\frac{1}{2}(z + z^{-1})) \) and note that \( g(z) \) is analytic in the annulus \( R^{-1} < |z| < R \). Hence, \( M(\rho) \) can be rewritten as

\[
M(\rho) = \frac{1}{\pi} \int_{0}^{2\pi} |g(\rho e^{i\theta})|d\theta.
\]

We further define \( |g(\rho e^{i\theta})| = g(\rho e^{i\theta})\phi(\rho, \theta) \) and

\[
F(z) = \frac{1}{\pi} \int_{0}^{2\pi} g(z e^{i\theta})\phi(\rho, \theta)d\theta.
\]

It is clear to see that \( F(z) \) is analytic in the annulus \( R^{-1} < |z| < R \). For \( 1 \leq \rho \leq r \) and \( 1 \leq r < R \), we restrict our attention to the annulus \( r^{-1} < |z| < r \). By the maximum modulus theorem, \( F(z) \) achieves its maximum modulus on the boundary \( |z| = r^{-1} \) or \( |z| = r \). More specifically, we suppose that \( F(z) \) achieves its maximum modulus at \( z = r^{-1}e^{i\theta_1} \) or \( F(z) = re^{i\theta_2} \). Therefore,

\[
M(\rho) = F(\rho) \leq \max \left\{ |F(r^{-1}e^{i\theta_1})|, |F(re^{i\theta_2})| \right\}
\]

\[
\leq \max \{ M(r^{-1}), M(r) \}
\]

\[
= M(r), \quad (3.16)
\]

where we have used the fact that \( |\phi(\rho, \theta)| = 1 \). This proves the second assertion. For the first and the third assertions, noting that Hardy’s proof given in [14] is still valid for functions \( g \) defined on an annulus region, these two assertions follow immediately. \( \square \)

Since \( \log \kappa_{Ch1}(n, \rho) = \log M(\rho) - \log |a_n| - n \log \rho \), we have the following corollary.

**Corollary 3.4.** Let \( f \) be analytic on and inside an ellipse \( E_\rho \) with \( 1 \leq \rho < R \). Then for each Chebyshev coefficient \( a_n \neq 0 \), we have

1. \( \kappa_{Ch1}(n, \rho) \) is continuously differentiable with respect to \( \rho \).

2. If \( f \) is not a constant, \( \log(\kappa_{Ch1}(n, \rho)) \) is a convex function of \( \log \rho \).

In the analysis of Bornemann, [4, Theorem 4.1] and [3, Corollary 4.2] are the key steps in proving that an optimal radius exists for Cauchy integrals of the form (1.1). Afterwards, it remains to analyze the limits \( r \to 0 \) and \( r \to \infty \). The limit \( r \to 0 \) is always unstable. The limit in the other direction depends on the analyticity properties of \( f \) in the complex plane.

With our analogous Theorem 3.3 and Corollary 3.4 at hand, we can reuse Bornemann’s results in the context of Chebyshev coefficients with only slight adjustments. One major difference concerns the difference between the limits for small \( \rho \) and \( r \). Indeed, contrary to the limit \( r \to 0 \) in the setting of Taylor series coefficients, there is no
numerical instability associated with the limit $\rho \to 1$. Recall also that $M(\rho) = M(\rho^{-1})$, so that we don’t consider the case $\rho < 1$. It is clear that $M(\rho)$ is bounded as $\rho \to 1$ and we have:

**Theorem 3.5.** Assume $f$ is analytic in any ellipse $E_\rho$ with $1 \leq \rho < R$ and let $a_n$ be nonzero. Then

$$
\lim_{\rho \to 1} \kappa_{Ch1}(n, \rho) = \frac{1}{\pi |a_n|} \int_0^{2\pi} |f(\cos \theta)| d\theta.
$$

**Proof.** This follows from the definitions (3.13) and (3.14). \qed

Two interesting results to formulate explicitly are as follows.

**Theorem 3.6.** Assume $f$ is an entire transcendental function and

$$
M(\rho) \sim e^{\mu \rho^\nu} \rho^{\varsigma}, \quad \rho \to \infty,
$$

where $\mu$ is positive and finite and $\nu$ is positive. Then, the optimal radius satisfies asymptotically

$$
\rho^*(n) \sim \left( \frac{n - \varsigma}{\mu \nu} \right)^{\frac{1}{\nu}}.
$$

**Proof.** For large $\rho$, we have the asymptotic behaviour of the condition number

$$
\kappa_{Ch1}(n, \rho) = \frac{M(\rho)}{|a_n| \rho^n} \sim \frac{e^{\mu \rho^\nu} \rho^{\varsigma - n}}{|a_n|} = \frac{1}{|a_n|} e^{\mu \rho^\nu + (\varsigma - n) \log \rho}.
$$

According to Theorem 3.3, we can simply differentiate the expression on the right hand side to derive an optimal value of $\rho$ such that the condition number $\kappa(n, \rho)$ is asymptotically minimized. This formal differentiation of an asymptotic formula is guaranteed to be valid in this case: for a rigorous discussion, we refer the reader to [4, Thm. 8.4]. Direct calculation shows that the above asymptotic expression on the right hand side takes its minimum value at $\rho = \left( \frac{n - \varsigma}{\mu \nu} \right)^{\frac{1}{\nu}}$. This completes the proof. \qed

Next, we consider the case where $f$ is only analytic in a bounded region in the complex plane. Define

$$
\vartheta = \sup_{1 < \rho < \rho_{\text{max}}} \frac{\rho M'(\rho)}{M(\rho)}.
$$

Furthermore, applying the third assertion of Theorem 3.3 we have

$$
\vartheta = \lim_{\rho \to \rho_{\text{max}}} \frac{\rho M'(\rho)}{M(\rho)}.
$$

The following theorem is analogous to [4, Thm. 4.5], which shows the optimal radius approaches $\rho_{\text{max}}$ for large $n$.  

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Theorem 3.7. Let \( f \) be analytic in any ellipse \( E_\rho \) with \( 1 \leq \rho < R < \infty \). Then,

1. If \( n > \vartheta \), the condition number \( \kappa^{\text{Ch}1}(n, \rho) \) is strictly decreasing for \( 1 < \rho < \rho_{\text{max}} \).
2. If \( \vartheta = \infty \), then \( \kappa^{\text{Ch}1}(n, \rho) \) is strictly increasing in the vicinity of \( \rho = \rho_{\text{max}} \).
3. If \( \vartheta < \infty \) and \( \lim_{\rho \to \rho_{\text{max}}} M(\rho) \) exists and is finite, then the optimal radius \( \rho = \rho_{\text{max}} \) for \( n > \vartheta \).

Proof. In analogy to \cite[Thm. 4.5]{4}, differentiating the condition number with respect to \( \rho \) yields

\[
\frac{d}{d\rho} \log \kappa^{\text{Ch}1}(n, \rho) = \frac{M'(\rho)}{M(\rho)} - \frac{n}{\rho} \leq \frac{\vartheta - n}{\rho}.
\]

If \( n > \vartheta \), then the condition number \( \kappa^{\text{Ch}1}(n, \rho) \) is a strictly decreasing function of \( \rho \) and the first assertion follows. If \( \vartheta = \infty \), this implies that \( \kappa^{\text{Ch}1}(n, \rho) \) is strictly increasing when \( \rho \to \rho_{\text{max}} \), thus the second assertion holds. Finally, if \( \vartheta < \infty \) and \( \lim_{\rho \to \rho_{\text{max}}} M(\rho) \) exists and is finite, then the third assertion follows from the first assertion.

### 3.4 Examples of optimal contours

In this section we give some specific examples of optimal radii. However, first we show that the condition number accurately predicts the relative error of the Chebyshev coefficients. Fig. 1 shows the condition number, as well as the ratio of the relative error of the Chebyshev coefficients to the machine precision, for two entire functions \( f(x) = e^x \) and \( f(x) = \cos(2x + 2) \). There is a clear agreement between both quantities. Fig. 2 shows the same experiment for two analytic functions that are not entire, \( f(x) = \frac{1}{x^2} \) and \( f(x) = \frac{x}{x^2 + 1} \). From this figure we observe that the condition number assumes its minimum value when \( \rho \) is close to its maximum value.

Example 3.8. Consider the exponential function \( f(x) = e^x \), which is entire and transcendental. Its Chebyshev coefficients are \( a_n = 2I_n(1) \) and

\[
\int_0^{2\pi} e^{\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})} d\theta = \int_0^{2\pi} e^{\frac{1}{2}(\rho + \rho^{-1}) \cos \theta} d\theta = 2\pi I_0(\frac{1}{2}(\rho + \rho^{-1})),
\]

where \( I_n(x) \) is the modified Bessel function of the first kind of order \( n \) \cite[p. 376]{1}. Thus, the condition number is

\[
\kappa^{\text{Ch}1}(n, \rho) = \frac{1}{I_n(1)} I_0(\frac{1}{2}(\rho + \rho^{-1})) \rho^{-n}. \tag{3.19}
\]

Using the first term of the asymptotic expansion of the \( I_n(x) \) \cite[p. 377]{1}

\[
I_n(x) = \frac{e^x}{\sqrt{2\pi x}} \left( 1 - \frac{4n^2 - 1}{8x} + O(x^{-2}) \right), \quad x \to \infty,
\]

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Figure 1: Ratio of the relative error of the $n$-th Chebyshev coefficients to the machine precision (dots) and the condition number $\kappa(n, \rho)$ (line) for $n = 20, 60$, respectively. The test functions are $f(x) = e^x$ (left) and $f(x) = \cos(2x + 2)$ (right).

we get from Theorem 3.6 that
\[ \mu = \frac{1}{2}, \quad \nu = 1, \quad \varsigma = \frac{1}{2}. \]

Therefore,
\[ \rho^*(n) = 2n + 1. \]

Direct calculation of the condition number yields
\[ 1 \leq \kappa_{\text{Ch1}}(n, 2n + 1) < 1.08, \quad n \geq 0. \]

This bound for condition number shows that the Chebyshev coefficients can be accurately computed without loss of accuracy if the optimal radius is used.

**Example 3.9.** Consider the cosine function $f(x) = \cos(cx + d)$ with real constants $c, d$ and $c > 0$. The exact Chebyshev coefficients are
\[ a_n = 2\cos \left( d + n\frac{\pi}{2} \right) J_n(c), \quad n \geq 0, \]
where $J_n(x)$ denotes the Bessel function of the first kind. We have
\begin{align*}
M(\rho) &= \frac{1}{\pi} \int_0^{2\pi} \left| \cos \left( \frac{c}{2}(\rho e^{i\theta} + (\rho e^{-i\theta})^{-1}) + d \right) \right| d\theta \\
&= \frac{1}{2\pi} \int_0^{2\pi} \sqrt{e^{c(\rho-\rho^{-1})\sin\theta} + e^{-c(\rho-\rho^{-1})\sin\theta} + 2\cos(c(\rho + \rho^{-1})\cos\theta + 2d)} d\theta \\
&= \frac{1}{\pi} \int_0^{\pi} \sqrt{e^{c(\rho-\rho^{-1})\sin\theta} + e^{-c(\rho-\rho^{-1})\sin\theta} + 2\cos(c(\rho + \rho^{-1})\cos\theta + 2d)} d\theta.
\end{align*}
Figure 2: Ratio of the relative error of the $n$-th Chebyshev coefficients to the machine precision (dots) and the condition number $\kappa(n, \rho)$ (line) for $n = 20, 60$, respectively. The test functions are $f(x) = \frac{1}{x^2}$ (left) and $f(x) = \frac{x + 1}{x^2 + 1}$ (right).

For large $\rho$, noting that the sum in the last equality is dominated by the first term, we have

$$M(\rho) \sim \frac{1}{\pi} \int_{0}^{\pi} e^{\frac{\pi}{2} (\rho^{-1} - \rho)} \sin \theta d\theta$$

$$= I_0 \left(\frac{c}{2} (\rho^{-1} - \rho)\right) + \frac{4}{\pi} \sum_{k=0}^{\infty} \frac{(-1)^k}{2k + 1} I_{2k+1} \left(\frac{c}{2} (\rho^{-1} - \rho)\right),$$

where we have made use of the expansion [1, Eqn. 9.6.35]. Using the first term of the asymptotic expansion of $I_n(x)$, we obtain

$$M(\rho) \sim 2 \frac{e^{\frac{\pi}{2} \rho}}{\sqrt{c \pi \rho}}, \quad \rho \to \infty.$$ 

Identifying with Theorem 3.6 leads to

$$\mu = \frac{c}{2}, \quad \nu = 1, \quad \varsigma = -\frac{1}{2}.$$ 

Thus, we can derive the optimal radius for the cosine function

$$\rho^*(n) = \frac{2n + 1}{c}.$$ 

For example, for $c = 2$ and $d = 2$, direct calculation shows

$$1 < \kappa^{Ch1}(n, \frac{2n + 1}{c}) < 2.48, \quad n \geq 1.$$
Example 3.10. Consider a model function with a simple pole on the real line

$$f(x) = \frac{1}{x - a},$$

where $a > 1$. The exact Chebyshev coefficients are given by \[\text{Eqn. (5.14)}\]

$$a_n = -\frac{2}{\sqrt{a^2 - 1}}(a - \sqrt{a^2 - 1})^n, \quad n \geq 0.$$  

Note that $f$ has a pole at $z = a$, we can deduce immediately that $1 < \rho < A$ and $A = a + \sqrt{a^2 - 1}$. Direct calculation gives

$$M(\rho) = \frac{1}{\pi} \int_0^{2\pi} \frac{1}{|\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) - a|} d\theta$$

$$= \frac{2\rho}{\pi} \int_0^{2\pi} \frac{1}{|((\rho e^{i\theta})^2 - 2a(\rho e^{i\theta}) + 1)|} d\theta$$

$$= \frac{2\rho}{\pi} \int_0^{2\pi} \frac{1}{|((\rho e^{i\theta} - A)(\rho e^{i\theta} - A^{-1})|} d\theta.$$  

The latter integral can be evaluated exactly in terms of elliptic integrals. An asymptotic expression for $\rho$ tending to $A$ is

$$M(\rho) \sim \frac{4\rho}{\pi} \frac{3 \log 2 + \log(A(A^2 - 1)) - \log(A^2 + 1) - \log(A - \rho)}{A^2 - 1}. $$

Optimizing the condition number for large $n$ leads, after further asymptotic approximations, to

$$\rho^*(n) = A \left(1 - \frac{1}{n(3 \log 2 + \log n)}\right).$$

For small values of $A$ and $n$, a slightly more accurate expression is

$$\rho^*(n) = A \left(1 - \frac{1}{n(3 \log 2 - \log(A^2 + 1) + \log(A^2 - 1) + \log n)}\right).$$

This leads for both expressions to a logarithmic growth of the condition number as a function of $n$, approximately $\log n/\pi$. Similar growth was observed for the computation of high derivatives of this function in \[\text{Example 5.2}\].

For example, when $a = 2$ direct calculation shows

$$1 < \kappa_{Ch1}(n, \rho^*(n)) < 4.72, \quad 0 \leq n \leq 10000,$$

if we choose the optimal radius

$$\rho^*(n) = \begin{cases} 
A \left(1 - \frac{1}{n(3 \log 2 + \log n)}\right), & \text{if } n \geq 1, \\
A \left(1 - \frac{1}{3 \log 2}\right), & \text{if } n = 0. 
\end{cases}$$  

(3.20)
The case where $f$ has a complex pole can be analyzed similarly, but is slightly more involved. Expression (3.20) for the optimal radius continues to hold for a pole at the point $z_0$, with
\[ A = |z_0 \pm \sqrt{z_0^2 - 1}| \]
and where the sign is chosen such that $A > 1$. We omit the details of the derivation.

**Remark 3.11.** In order to achieve the relative error tolerance $\epsilon$ by using the optimal radius, numerical experiments suggest that we need about
\[ m_\epsilon \approx n(3 \log 2 + \log n) \log \epsilon^{-1} \]
(3.21) nodes for large $n$. For example, we consider the computation of $a_{100}$ of the function $f(x) = \frac{1}{x}$. To achieve relative error $\epsilon = 10^{-13}$, we need $m_\epsilon \approx 20009$ nodes. Numerical results show that the relative error is $2 \times 10^{-14}$ when $m = 20010$.

**Example 3.12.** Consider the function
\[ f(x) = (c - x)^{\phi} g(x), \]
where $\phi > 0$ is not an integer and $c > 1$ and $g(x)$ is an analytic function at $x = c$. In this example, $f(x)$ has a branch point at $x = c$. Direct calculations show that the maximum value of $\rho$ is
\[ \rho_{\text{max}} = c + \sqrt{c^2 - 1} \quad \text{and} \quad M(\rho) = \frac{1}{\pi} \int_0^{2\pi} \left| f\left(\frac{1}{2}(\rho e^{i\theta}) + (\rho e^{i\theta})^{-1}\right) \right| d\theta \]
\[ = \frac{1}{\pi} \int_0^{2\pi} \left| \left( c - \frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) \right)^{\phi} g\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) \right| d\theta \]
\[ = \frac{1}{\pi} \int_0^{2\pi} \left| \frac{1}{4}(\rho^2 + \rho^{-2}) - c(\rho + \rho^{-1}) \cos \theta + \frac{1}{2} \cos(2\theta) + c^2 \right|^{\frac{\phi}{2}} \left| g\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) \right| d\theta. \]
(3.22)
It is easy to see that the integral in the last equation is bounded when $\rho = \rho_{\text{max}}$. Applying Theorem 3.3 we have
\[ \lim_{\rho \to \rho_{\text{max}}} \kappa^{\text{Ch}1}(n, \rho) = \lim_{\rho \to \rho_{\text{max}}} \frac{M(\rho)}{|a_n|\rho_{\text{max}}^n}, \]
and the limit is finite. Thus, from Theorem 3.7 we deduce that the optimal radius is $\rho^*(n) = \rho_{\text{max}}$ for large $n$. Moreover, from [12 Eqn. (37)] we know that the Chebyshev coefficients of $f(x)$ have the following estimate
\[ a_n \simeq -\frac{2 \sin(\phi \pi)(c^2 - 1)^{\frac{\phi}{2}}g(c)\Gamma(\phi + 1)}{\pi n^{\phi+1}\rho_{\text{max}}^n}. \]
Thus, we can estimate the growth of the optimal condition number
\[ \kappa^{\text{Ch}1}(n, \rho^*(n)) = \frac{M(\rho)}{|a_n|\rho_{\text{max}}^n} \sim \mathcal{O}(n^{\phi+1}), \quad n \to \infty, \]
which shows the optimal condition number grows algebraically as $n \to \infty$. 

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3.5 Identifying Chebyshev coefficients with Taylor coefficients

An alternative way to reuse the results of [1] is to put the integral representation of the Chebyshev coefficients \[ \sum_{k=0}^{\infty} a_k T_k(x) \] into the form of a Cauchy integral like (1.1). We will show that this can be achieved by a conformal map. The main advantage is that theoretical results can be reused. However, this identification between integrals does not seem to lead to a new or improved numerical scheme.

Let us first show that the Chebyshev coefficients of an analytic function can be viewed as the Taylor coefficients of another analytic function. An explicit form of this function can be established in terms of a contour integral of \( f(z) \).

**Theorem 3.13.** Suppose that \( a_k \) are the Chebyshev coefficients of the first kind of the function \( f(z) \) which is analytic inside and on the ellipse \( E_\rho \). Then they are the Taylor coefficients of the following function

\[
H(x) = \frac{1}{\pi i} \oint_{C_\rho} \frac{f\left(\frac{1}{2}(u + u^{-1})\right)}{u - x} \, du,
\]

and \( H(x) \) is analytic inside the circle \( C_\rho \).

**Proof.** Suppose \( a_k \) are the Chebyshev coefficients of \( f \) and meanwhile the Taylor coefficients of another function \( H(x) \), e.g.

\[
f(x) = \sum_{k=0}^{\infty} a_k T_k(x), \quad H(x) = \sum_{k=0}^{\infty} a_k x^k.
\]

In view of the contour integral expression of \( a_k \), we have

\[
H(x) = \sum_{k=0}^{\infty} a_k x^k
\]

\[
= \frac{1}{\pi i} \oint_{C_\rho} f(z) \sum_{k=0}^{\infty} x^k u^{-k-1} \, du
\]

\[
= \frac{1}{\pi i} \oint_{C_\rho} f(z) \frac{du}{u - x}
\]

\[
= \frac{1}{\pi i} \oint_{C_\rho} f\left(\frac{1}{2}(u + u^{-1})\right) \frac{(1 - u^{-2})du}{u - x}. \tag{3.24}
\]

This completes the proof. \( \square \)

**Corollary 3.14.** Suppose that \( b_k \) are the Chebyshev coefficients of the second kind of the function \( f(z) \) which is analytic inside and on the ellipse \( E_\rho \), then they are the Taylor coefficients of the following function

\[
H(x) = \frac{1}{2\pi i} \oint_{C_\rho} \frac{f\left(\frac{1}{2}(u + u^{-1})\right)}{u - x} (1 - u^{-2}) \, du,
\]

and \( H(x) \) is analytic inside the circle \( C_\rho \).
In the following we present some concrete examples, where $H(x)$ can be deduced in (almost) closed form.

**Example 3.15.** Consider the exponential function $f(x) = e^x$. We have

$$H(x) = \frac{1}{\pi i} \oint_{C_\rho} e^{\frac{1}{2}(u+u^{-1})} \frac{1}{u-x} \, du.$$  \hspace{1cm} (3.26)

Direct calculations show that

$$a_k = H^{(k)}(0) = \frac{1}{k!} \oint_{C_\rho} e^{\frac{1}{2}(u+u^{-1})} \frac{1}{(u-x)^{k+1}} \, du$$

$$= \sum_{m=0}^{\infty} \frac{2^{k+2m} \Gamma(k+m+1) \Gamma(m+1)}{2^{2k+2m} \Gamma(k+m+1) \Gamma(m+1)}$$

$$= 2 I_k(1).$$  \hspace{1cm} (3.27)

Thus, we have

$$H(x) = \frac{2}{\pi i} \sum_{k=0}^{\infty} I_k(1) x^k,$$

which is an entire function.

**Example 3.16.** Consider the function

$$f(x) = \frac{1}{x-a}, \quad a > 1.$$  

Using the residue theorem, we obtain

$$H(x) = \frac{1}{\pi i} \oint_{C_\rho} \frac{f(\frac{1}{2}(u+u^{-1}))}{u-x} \, du$$

$$= \frac{1}{\pi i} \oint_{C_\rho} \frac{2u}{u^2 - 2au + 1} \frac{1}{u-x} \, du$$

$$= \frac{2(a + \sqrt{a^2 - 1})}{(x - (a + \sqrt{a^2 - 1})) \sqrt{a^2 - 1}}$$  \hspace{1cm} (3.28)

and $H(x)$ is analytic inside the circle $|z| < a + \sqrt{a^2 - 1}$.

### 4 Two strategies for computing the Chebyshev coefficients

In this section we present two strategies for computing the first $N + 1$ Chebyshev coefficients of analytic functions. The first strategy maximizes the computational efficiency and can be performed via the FFT. The second strategy minimizes the loss of accuracy for each coefficient and is stable with respect to relative errors.
4.1 Fast algorithms to maximize the efficiency

Note that the sum (3.1) for the computation of \( \{a_k\}_{k=0}^{N} \) is suitable for using FFT if \( \rho \) is fixed for all \( \{a_k(m, \rho)\}_{k=0}^{N} \). Therefore, by choosing the same value of \( \rho \) for each expansion coefficient, either for integral (3.1) or integral (3.4), the Chebyshev coefficients \( a_n \) and \( b_n \) can be computed efficiently with a single FFT and this process can be performed in \( O(m \log m) \) operations. In the following we present some numerical experiments to show the performance of the FFT algorithm.

**Example 4.1.** First, we consider the transcendental function \( f(x) = e^x \). Clearly, this function is entire and thus \( 1 \leq \rho < \infty \). In Figure 3 we show the absolute and relative errors of the FFT algorithm for computing the first \( N + 1 \) Chebyshev coefficients. We see that the absolute errors are uniformly small for \( 0 \leq k \leq N \) when we choose \( \rho = 1 \). When \( \rho > 1 \), we see that the absolute errors decrease exponentially as \( k \) increases. However, we also observe that the absolute errors deteriorate for the first several Chebyshev coefficients if \( \rho = 40 \). As for the relative error, we observe that it has the fastest rate of exponential growth when \( \rho = 1 \) and then becomes better as \( \rho \) increases. When \( \rho = 40 \), we see that the relative error deteriorates for the first several Chebyshev coefficients.

![Figure 3: Absolute errors (left) and relative errors (right) of the computed Chebyshev coefficients \( \{a_k(m, \rho)\}_{k=0}^{N} \) for the function \( f(x) = e^x \). Here we choose \( N = 50 \) and \( m = 2N + 1 \).](image)

**Example 4.2.** We consider the function \( f(x) = \frac{1}{x-2} \). Note that this function has a real pole at \( x = 2 \) and we can deduce that \( 1 \leq \rho < 2 + \sqrt{3} \approx 3.732 \). In our computations we choose \( m = 4N + 2 \) and we have tested several values of \( \rho \). Numerical results are presented in Figure 4. We see that, similar to the above example, the absolute errors are also uniformly small when we choose \( \rho = 1 \) and decrease exponentially as \( k \) increases when \( \rho > 1 \). As for the relative error, we observe that it grows exponentially with the fastest rate when \( \rho = 1 \) and then becomes better as \( \rho \) grows. In particular, the relative
error is less than $10^{-11}$ for all $\{a_k\}_{k=0}^N$ when $\rho = 3$. We point out that the absolute and relative errors will deteriorate simultaneously when $\rho$ is very close to its maximum value. This is due to the fact that the term $\|f - s_m\|_{\mathcal{E}_\rho}$ in Theorem 3.1 tends to infinity when $m$ is fixed and $\rho$ tends to its maximum value.

Finally, we conclude this subsection with several remarks.

**Remark 4.3.** For transcendental functions, the computation of their Chebyshev coefficients by a single $\rho$ may suffer from instability when $\rho \gg 1$.

**Remark 4.4.** Numerical experiments show that, for a fixed $\rho$, it is sufficient to choose $m = \mathcal{O}(N)$ such that the absolute errors of the first $N+1$ Chebyshev coefficients are less than a given tolerance uniformly. Thus the cost is $\mathcal{O}(N \log N)$ operations for computing the first $N+1$ Chebyshev expansion coefficients.

**Remark 4.5.** If we are concerned only with the absolute errors of Chebyshev coefficients, it is sufficient to choose $\rho = 1$ and $m = \mathcal{O}(N)$. This leads to a fast algorithm which costs only $\mathcal{O}(N \log N)$ operations for computing the first $N+1$ Chebyshev coefficients. However, if we are concerned with the relative errors, the situation will change completely and it is dangerous to choose $\rho = 1$ since they have the fastest rate of exponential growth.

**Remark 4.6.** If $f(x)$ is analytic only in a neighborhood of $[-1, 1]$, it is possible to compute all Chebyshev coefficients $\{a_k\}_{k=0}^N$ by choosing a single $\rho$ such that their relative errors are less than a given tolerance.

### 4.2 Maximizing the accuracy of Chebyshev coefficients

We can see from the above subsection that the relative errors of Chebyshev coefficients may grow exponentially as $k$ grows if we compute them by using the same $\rho$. To remedy
this drawback, we propose an alternative strategy and compute each Chebyshev coefficient $a_k$ by using its optimal $\rho^*(k)$. This leads to an accurate algorithm which minimizes the loss of accuracy with respect to relative errors.

In Figure 5 we show relative errors of this strategy for computing the first $N + 1$ Chebyshev coefficients of the functions $f(x) = e^x$, $\frac{1}{x^2}$. For the former function, each Chebyshev coefficient $a_k$ is computed by (3.1) with $\rho = 2k + 1$ and $m = 2N + 1$. For the latter function, each Chebyshev coefficient $a_k$ is evaluated by the trapezoidal rule (3.1) with the optimal radius (3.20) and the number of points in the trapezoidal rule is chosen as

$$m = \max\{k(3 \log 2 + \log k) \log \epsilon^{-1}, 50\}, \quad 0 \leq k \leq 100,$$

and we choose $\epsilon = 10^{-14}$. We can see that the Chebyshev coefficients can be evaluated very accurately with respect to relative errors.

![Figure 5: Relative errors of the computed Chebyshev coefficients $\{a_k(m, \rho^*(k))\}_{k=0}^N$ of $f(x) = e^x$ (left) and $f(x) = \frac{1}{x^2}$ (right). Here $N = 100$.](image)

Bornemann analyzes the number of quadrature points $m$ to use for the computation of the Taylor coefficient $a_n$ in terms of $n$, and this depends on the nature of the function, in particular its analyticity properties [4, §2]. We found experimentally that these results can be reused in the setting of the computation of Chebyshev coefficients, and this has guided the choice of $m$ for the examples in the current paper.

5 Chebyshev spectral differentiation

In this section we show some examples to illustrate the accuracy of Chebyshev spectral differentiation based on the spectral expansions. Let

$$f_N^c(x) = \sum_{k=0}^N \tilde{a}_k T_k(x)$$
denote the truncated Chebyshev expansion. Then the derivatives of \( f(x) \) can be approximated by the corresponding derivatives of \( f_N^{(s)}(x) \), e.g.
\[
f^{(s)}(x) \approx \frac{d^s}{dx^s} f_N^{(s)}(x).
\]
Let
\[
\frac{d^s}{dx^s} f_N^{(s)}(x) = \sum_{k=0}^{N-s} a_k^{(s)} T_k(x).
\]
Then the coefficients \( a_k^{(s)} \) can be evaluated by using the following recurrence relation [5, p. 498]
\[
a_{k-1}^{(s)} = a_{k+1}^{(s)} + 2k a_k^{(s-1)}, \quad k = N - s + 1, \ldots, 1, \tag{5.1}
\]
where \( a_{N-s+2}^{(s)} = a_{N-s+1}^{(s)} = 0 \). Moreover, the initial coefficients are given by \( a_k^{(0)} = a_k \) for \( 0 \leq k \leq N \).

**Example 5.1.** We consider the accuracy of the Chebyshev spectral differentiation for the test function \( f(x) = e^x \). Each Chebyshev coefficient \( a_k \) is evaluated by the trapezoidal rule (3.1) with the optimal radius and the number of points in the trapezoidal rule is \( m = 100 \). In Figure 6 we present the pointwise errors in the evaluation of the \( s \)-th order derivative of \( f(x) \) by the truncated Chebyshev spectral expansion \( f_N^{(s)}(x) \). The error is measured at 100 equispaced points in \([-1, 1]\). As can be seen, the error of the Chebyshev spectral differentiation is always very close to machine precision.

![Figure 6](image_url)

**Figure 6:** Errors of the \( s \)-th order derivative of the truncated Chebyshev expansion \( f_N^{(s)}(x) \). Here we choose \( N = 100 \) and \( s = 5 \) (left), \( s = 20 \) (middle) and \( s = 80 \) (right).

**Example 5.2.** We consider the accuracy of the Chebyshev spectral differentiation for the function \( f(x) = \cos(x) \). Each Chebyshev coefficient \( a_k \) is evaluated by the trapezoidal rule (3.1) with the optimal radius and the number of points in the trapezoidal rule is \( m = 100 \). In Figure 7 we present the pointwise errors in the evaluation of the \( s \)-th order derivative of \( f(x) \) by the truncated Chebyshev spectral expansion \( f_N^{(s)}(x) \).
Figure 7: Errors of the s-th order derivative of the truncated Chebyshev expansion $f_N^C(x)$. Here we choose $N = 100$ and $s = 10$ (left), $s = 40$ (middle) and $s = 80$ (right).

Example 5.3. Finally, we consider the accuracy of the Chebyshev spectral differentiation for the test function $f(x) = \frac{x+1}{x^2+4}$. Each Chebyshev coefficient $a_k$ is evaluated by the trapezoidal rule (3.1) with the optimal radius and the number of points in the trapezoidal rule is chosen as

$$m = \max\{n(3 \log 2 + \log n) \log \epsilon^{-1}, 50\}, \quad 0 \leq n \leq 100,$$

and we choose $\epsilon = 10^{-16}$. The pointwise error of the Chebyshev spectral differentiation in the evaluation of the s-th order derivative of $f(x)$ is displayed in Figure 8.

Figure 8: Errors of the s-th order derivative of the truncated Chebyshev expansion $f_N^C(x)$. Here we choose $N = 100$ and $s = 4$ (left), $s = 8$ (middle) and $s = 12$ (right).

6 Computing the roots of derivatives of analytic functions

One powerful application of the truncated Chebyshev expansion of an analytic function $f(x)$ is that it can be used to compute the roots of $f(x)$ on the interval $[-1, 1]$. The main idea is that the roots of a Chebyshev series are the eigenvalues of a colleague matrix.
whose elements are simple functions of the coefficients of the Chebyshev series. For the sake of clarity, we state it in the following.

**Theorem 6.1.** The roots of the Chebyshev series

\[ p(x) = \sum_{k=0}^{n} c_k T_k(x), \quad c_n \neq 0, \]

are the eigenvalues of the following colleague matrix

\[ A = \begin{pmatrix} 0 & 1 & \frac{1}{2} & 0 & \frac{1}{2} & \cdots & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \frac{1}{2} & \cdots & \frac{1}{2} \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \frac{1}{2} & \cdots & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \frac{1}{2} & \cdots & \frac{1}{2} \\ \end{pmatrix} - \frac{1}{2c_n} \begin{pmatrix} c_0 & c_1 & c_2 & \cdots & c_{n-1} \\ \end{pmatrix}. \] (6.1)

If there are multiple roots, these correspond to eigenvalues with the same multiplicities.

*Proof.* See [25, Thm. 18.1].

In practice, it is of particular interest to compute the roots of derivatives of a smooth function. For example, the roots of the first and second order derivatives of a function correspond exactly to its maxima and inflexion points. In the following, we show the performance of our methods applied to the computation of derivatives of a transcendental function. As shown in the above section, the Chebyshev coefficients of the \( s \)-th order derivatives of \( f_C(x) \) can be computed via the recurrence relation (5.1) and thus the roots of \( \frac{df}{dx^s} f_C(x) \) can be computed by using Theorem 6.1.

**Example 6.2.** Consider

\[ f(x) = e^{2x} + \cos(2x + 3), \quad x \in [-1, 1], \]

For each Chebyshev coefficient \( a_n \) of \( f(x) \), it is not difficult to deduce that the optimal radius is \( \rho^*(n) = n + \frac{1}{2} \). In the following we present several numerical results on the computation of \( s \)-th order derivative of \( f(x) \). For comparison, we perform the computations with two different approaches when compute the Chebyshev coefficients of \( f(x) \):  

1. We compute each \( a_k \) by using its optimal radius \( \rho^*(k) \);

2. We compute all \( a_k \) by choosing the same radius \( \rho = 1 \) (we use the sample points of \( f(x) \) on the interval \([-1, 1])

In our computations, each \( a_k \) is evaluated by using the trapezoidal rule with \( m = 100 \). Numerical results are presented in Figure 9. As can be seen, our approach is advantageous when we compute the roots of derivatives. In Figure 10 we illustrate the results for the roots of higher order derivatives.
7 Conclusion

In this paper, we have discussed the computation of Chebyshev expansion coefficients of analytic functions. Two strategies have been proposed based on the computational accuracy and efficiency of the Chebyshev expansion coefficients. The first strategy is that we compute all Chebyshev coefficients using the same contour and this process can be performed efficiently via the FFT. However, this strategy may not be stable with respect to relative errors. Alternatively, we propose the second strategy by extending the idea of Bornemann’s analysis for the Taylor coefficients to the Chebyshev coefficients. We show that an optimal contour exists for each Chebyshev expansion coefficient. Computing each Chebyshev expansion coefficient with the optimal radius guarantees the relative error to be small. We further applied the second strategy to compute derivatives of analytic functions by differentiating the Chebyshev expansion. Numerical experiments show that this strategy provides very accurate approximation even for very high order derivatives. Finally, we apply this strategy to compute the roots of derivatives of analytic functions.

The main focus of this paper has been to investigate the benefits of computing Chebyshev coefficients in the complex plane. Several questions remain, and are topic of further research:

- Can the optimal radius be deduced automatically and numerically?
- What is an appropriate number of quadrature points to use along the contour in the complex plane, for a given radius and a given coefficient $a_n$?
Figure 10: Errors of the root of the \( s \)th order derivative of the truncated Chebyshev expansion \( f_N'(x) \) for \( s = 4 \) (left) and \( s = 5 \) (right). The dots denote the results of the strategy that each \( a_k \) is evaluated by the \( \rho^s(k) \) and the circles denote the strategy that all \( \{a_k\}_{k=0}^N \) are computed by setting \( \rho = 1 \).

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