

## Chapter 3

# Chebyshev Expansions

*The best is the cheapest.*  
—Benjamin Franklin

### 3.1 Introduction

In Chapter 2, approximations were considered consisting of expansions around a specific value of the variable (finite or infinite); both convergent and divergent series were described. These are the preferred approaches when values around these points (either in  $\mathbb{R}$  or  $\mathbb{C}$ ) are needed.

In this chapter, approximations in real intervals are considered. The idea is to approximate a function  $f(x)$  by a polynomial  $p(x)$  that gives a uniform and accurate description in an interval  $[a, b]$ .

Let us denote by  $\mathbb{P}_n$  the set of polynomials of degree at most  $n$  and let  $g$  be a bounded function defined on  $[a, b]$ . Then the uniform norm  $\|g\|$  on  $[a, b]$  is given by

$$\|g\| = \max_{x \in [a, b]} |g(x)|. \quad (3.1)$$

For approximating a continuous function  $f$  on an interval  $[a, b]$ , it is reasonable to consider that the best option consists in finding the *minimax approximation*, defined as follows.

**Definition 3.1.**  $q \in \mathbb{P}_n$  is the best (or minimax) polynomial approximation to  $f$  on  $[a, b]$  if

$$\|f - q\| \leq \|f - p\| \quad \forall p \in \mathbb{P}_n. \quad (3.2)$$

Minimax polynomial approximations exist and are unique (see [152]) when  $f$  is continuous, although they are not easy to compute in general. Instead, it is a more effective approach to consider near-minimax approximations, based on Chebyshev polynomials.

Chebyshev polynomials form a special class of polynomials especially suited for approximating other functions. They are widely used in many areas of numerical analysis: uniform approximation, least-squares approximation, numerical solution of ordinary and partial differential equations (the so-called spectral or pseudospectral methods), and so on.

In this chapter we describe the approximation of continuous functions by Chebyshev interpolation and Chebyshev series and how to compute efficiently such approximations. For the case of functions which are solutions of linear ordinary differential equations with polynomial coefficients (a typical case for special functions), the problem of computing Chebyshev series is efficiently solved by means of Clenshaw's method, which is also presented in this chapter.

Before this, we give a very concise overview of well-known results in interpolation theory, followed by a brief summary of important properties satisfied by Chebyshev polynomials.

### 3.2 Basic results on interpolation

Consider a real function  $f$  that is continuous on the real interval  $[a, b]$ . When values of this function are known at a finite number of points  $x_i$ , one can consider the approximation by a polynomial  $P_n$  such that  $f(x_i) = P_n(x_i)$ . The next theorem gives an explicit expression for the lowest degree polynomial (the *Lagrange interpolation polynomial*) satisfying these interpolation conditions.

**Theorem 3.2 (Lagrange interpolation).** *Given a function  $f$  that is defined at  $n + 1$  points  $x_0 < x_1 < \dots < x_n \in [a, b]$ , there exists a unique polynomial of degree smaller than or equal to  $n$  such that*

$$P_n(x_i) = f(x_i), \quad i = 0, \dots, n. \quad (3.3)$$

*This polynomial is given by*

$$P_n(x) = \sum_{i=0}^n f(x_i) L_i(x), \quad (3.4)$$

*where  $L_i(x)$  is defined by*

$$L_i(x) = \frac{\pi_{n+1}(x)}{(x - x_i)\pi'_{n+1}(x_i)} = \frac{\prod_{j=0, j \neq i}^n (x - x_j)}{\prod_{j=0, j \neq i}^n (x_i - x_j)}, \quad (3.5)$$

$\pi_{n+1}(x)$  being the nodal polynomial,  $\pi_{n+1}(x) = \prod_{j=0}^n (x - x_j)$ .

*Additionally, if  $f$  is continuous on  $[a, b]$  and  $n + 1$  times differentiable in  $(a, b)$ , then for any  $x \in [a, b]$  there exists a value  $\zeta_x \in (a, b)$ , depending on  $x$ , such that*

$$R_n(x) = f(x) - P_n(x) = \frac{f^{n+1}(\zeta_x)}{(n + 1)!} \pi_{n+1}(x). \quad (3.6)$$

**Proof.** The proof of this theorem can be found elsewhere [45, 48].  $\square$

$L_i$  are called the *fundamental Lagrange interpolation polynomials*.

The first part of the theorem is immediate and  $P_n$  satisfies the interpolation conditions, because the polynomials  $L_i$  are such that  $L_i(x_j) = \delta_{ij}$ . The formula for the remainder can be proved from repeated application of Rolle's theorem (see, for instance, [48, Thm. 3.3.1]).

For the particular case of Lagrange interpolation over  $n$  nodes, a simple expression for the interpolating polynomial can be given in terms of *forward differences* when the nodes are equally spaced, that is,  $x_{i+1} - x_i = h$ ,  $i = 0, \dots, n - 1$ . In this case, the interpolating polynomials of Theorem 3.2 can be written as

$$P_n(x) = \sum_{i=0}^n \binom{s}{i} \Delta^i f_0, \quad (3.7)$$

where

$$s = \frac{x - x_0}{h}, \quad \binom{s}{i} = \frac{1}{i!} \prod_{j=0}^{i-1} (s - j), \quad f_j = f(x_j), \quad (3.8)$$

$$\Delta f_j = f_{j+1} - f_j, \quad \Delta^2 f_j = \Delta(f_{j+1} - f_j) = f_{j+2} - 2f_{j+1} + f_j, \dots$$

This result is easy to prove by noticing that  $f_s = (\Delta + I)^s f_0$ ,  $s = 0, 1, \dots, n$ , and by expanding the binomial of commuting operators  $\Delta$  and  $I$  ( $I$  being the identity,  $If_i = f_i$ ).

The formula for the remainder in Theorem 3.2 resembles that for the Taylor formula of degree  $n$  (Lagrange form), except that the nodal polynomials in the latter case contain only one node,  $x_0$ , which is repeated  $n + 1$  times (in the sense that the power  $(x - x_0)^{n+1}$  appears). This interpretation in terms of *repeated nodes* can be generalized; both the Taylor formula and the Lagrange interpolation formula can be seen as particular cases of a more general interpolation formula, which is *Hermite interpolation*.

**Theorem 3.3 (Hermite interpolation).** *Let  $f$  be  $n$  times differentiable with continuity in  $[a, b]$  and  $n + 1$  times differentiable in  $(a, b)$ . Let  $x_0 < x_1 < \dots < x_k \in [a, b]$ , and let  $n_i \in \mathbb{N}$  such that  $n_0 + n_1 + \dots + n_k = n - k$ . Then, there exists a unique polynomial  $P_n$  of degree not larger than  $n$  such that*

$$P_n^{(j)}(x_i) = f^{(j)}(x_i), \quad j = 0, \dots, n_i, \quad i = 0, \dots, k. \quad (3.9)$$

Furthermore, given  $x \in [a, b]$ , there exists a value  $\zeta_x \in (a, b)$  such that

$$f(x) = P_n(x) + \frac{f^{n+1}(\zeta_x)}{(n+1)!} \pi_{n+1}(x), \quad (3.10)$$

where  $\pi_{n+1}(x)$  is the nodal polynomial

$$\pi_{n+1}(x) = (x - x_0)^{n_0+1} \dots (x - x_k)^{n_k+1} \quad (3.11)$$

in which each node  $x_i$  is repeated  $n_i + 1$  times.

**Proof.** For the proof we refer to [45].  $\square$

An explicit expression for the interpolating polynomial is, however, not so easy as for Lagrange's case. A convenient formalism is that of *Newton's divided difference formula*, also for Lagrange interpolation (see [45] for further details).

For the case of a single interpolation node  $x_0$  which is repeated  $n$  times, the corresponding interpolating polynomial is just the Taylor polynomial of degree  $n$  at  $x_0$ . It is very common that successive derivatives of special functions are known at a certain point  $x = x_0$  (Taylor's theorem, (2.1)), but it is not common that derivatives are known at several points. Therefore, in practical evaluation of special functions, Hermite interpolation different from the Taylor case is seldom used.

Lagrange interpolation is, however, a very frequently used method of approximation and, in addition, will be behind the quadrature methods to be discussed in Chapter 5. For interpolating a function in a number of nodes, we need, however, to know the values which the function takes at these points. Therefore, in general we will need to rely on an alternative (high-accuracy) method of evaluation.

However, for functions which are solutions of a differential equation, Clenshaw's method (see §3.6.1) provides a way to compute expansions in terms of Chebyshev polynomials. Such infinite expansions are related to a particular and useful type of Lagrange interpolation that we discuss in detail in §3.6.1 and introduce in the next section.

### 3.2.1 The Runge phenomenon and the Chebyshev nodes

Given a function  $f$  which is continuous on  $[a, b]$ , we may try to approximate the function by a Lagrange interpolating polynomial.

We could naively think that as more nodes are considered, the approximation will always be more accurate, but this is not always true. The main question to be addressed is whether the polynomials  $P_n$  that interpolate a continuous function  $f$  in  $n + 1$  equally spaced points are such that

$$\lim_{n \rightarrow \infty} \|f - P_n\| = \lim_{n \rightarrow \infty} \|R_n\| = 0, \quad (3.12)$$

where, if  $f$  is sufficiently differentiable, the error can be estimated through (3.6).

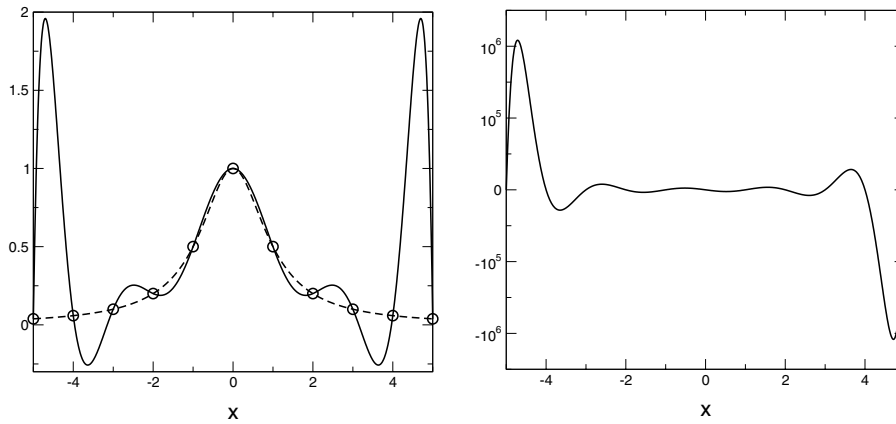
A pathological example for which the Lagrange interpolation does not converge is provided by  $f(x) = |x|$  in the interval  $[-1, 1]$ , for which equidistant interpolation diverges for  $0 < |x| < 1$  (see [189, Thm. 4.7]), as has been proved by Bernstein.

A less pathological example, studied by Runge, showing the *Runge phenomenon*, gives a clear warning on the problems of equally spaced nodes. Considering the problem of interpolation of

$$f(x) = \frac{1}{1 + x^2} \quad (3.13)$$

on  $[-5, 5]$ , Runge observed that  $\lim_{n \rightarrow \infty} \|f - P_n\| = \infty$ , but that convergence takes place in a smaller interval  $[-a, a]$  with  $a \simeq 3.63$ .

This bad behavior in Runge's example is due to the values of the nodal polynomial  $\pi_{n+1}(x)$ , which tends to present very strong oscillations near the endpoints of the interval (see Figure 3.1).



**Figure 3.1.** Left: the function  $f(x) = 1/(1+x^2)$  is plotted in  $[-5, 5]$  together with the polynomial of degree 10 which interpolates  $f$  at  $x = 0, \pm 1, \pm 2, \pm 3, \pm 4, \pm 5$ . Right: the nodal polynomial  $\pi(x) = x(x-1)(x-4)(x-9)(x-16)(x-25)$ .

The uniformity of the error in the interval of interpolation can be considerably improved by choosing the interpolation nodes  $x_i$  in a different way. Without loss of generality, we will restrict our study to interpolation on the interval  $[-1, 1]$ ; the problem of interpolating  $f$  with nodes  $x_i$  in the finite interval  $[a, b]$  is equivalent to the problem of interpolating  $g(t) = f(x(t))$ , where

$$x(t) = \frac{a+b}{2} + \frac{b-a}{2}t \quad (3.14)$$

with nodes  $t_i \in [-1, 1]$ .

Theorem 3.4 explains how to choose the nodes in  $[-1, 1]$  in order to minimize uniformly the error due to the nodal polynomial and to quantify this error. The nodes are given by the zeros of a Chebyshev polynomial.

**Theorem 3.4.** Let  $x_k = \cos((k+1/2)\pi/(n+1))$ ,  $k = 0, 1, \dots, n$ . Then the monic polynomial  $\hat{T}_{n+1}(x) = \prod_{k=0}^n (x - x_k)$  is the polynomial of degree  $n+1$  with the smallest possible uniform norm (3.1) in  $[-1, 1]$  in the sense that

$$\|\hat{T}_{n+1}\| \leq \|q_{n+1}\| \quad (3.15)$$

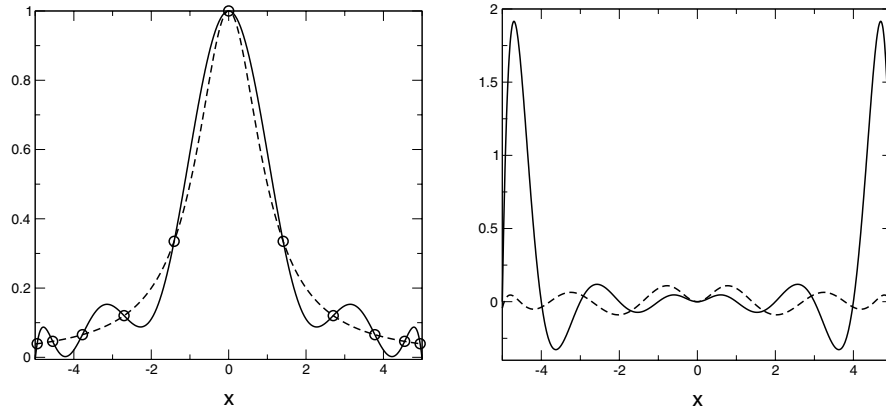
for any other monic polynomial  $q_{n+1}$  of degree  $n+1$ . Furthermore,

$$\|\hat{T}_{n+1}\| = 2^{-n}. \quad (3.16)$$

The selection of these nodes will not guarantee convergence as the number of nodes tends to infinity, because it also depends on how the derivatives of the function  $f$  behave, but certainly enlarges the range of functions for which convergence takes place and eliminates the problem for the example provided by Runge. Indeed, taking as nodes

$$x_k = 5 \cos((k+1/2)\pi/11), \quad k = 0, 1, \dots, 10, \quad (3.17)$$

instead of the 11 equispaced points, the behavior is much better, as illustrated in Figure 3.2.



**Figure 3.2.** Left: the function  $f(x) = 1/(1 + x^2)$  is plotted together with the interpolation polynomial for the 11 Chebyshev points (see (3.17)). Right: the interpolation errors for equispaced points and Chebyshev points is shown.

Before proving Theorem 3.4 and further results, we summarize the basic properties of Chebyshev polynomials, the zeros of which are the nodes in Theorem 3.4.

### 3.3 Chebyshev polynomials: Basic properties

Let us first consider a definition and some properties of the Chebyshev polynomials of the first kind.

**Definition 3.5 (Chebyshev polynomial of the first kind  $T_n(x)$ ).** The Chebyshev polynomial of the first kind of order  $n$  is defined as follows:

$$T_n(x) = \cos [n \cos^{-1}(x)], \quad x \in [-1, 1], \quad n = 0, 1, 2, \dots \quad (3.18)$$

From this definition the following property is evident:

$$T_n(\cos \theta) = \cos (n\theta), \quad \theta \in [0, \pi], \quad n = 0, 1, 2, \dots \quad (3.19)$$

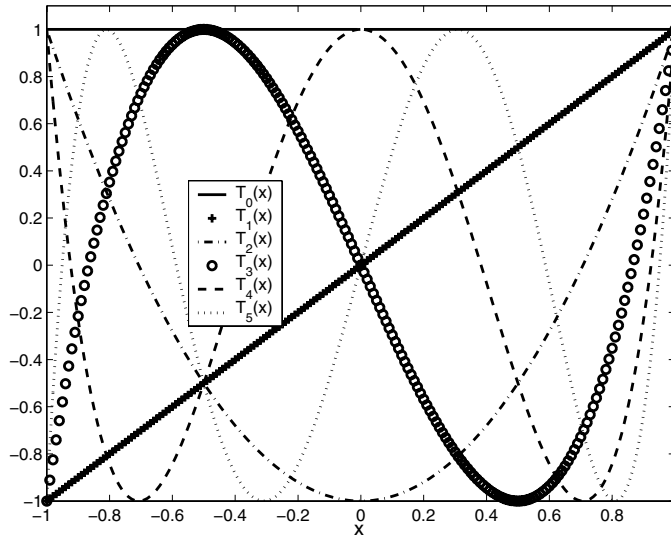
#### 3.3.1 Properties of the Chebyshev polynomials $T_n(x)$

The polynomials  $T_n(x)$ ,  $n \geq 1$ , satisfy the following properties, which follow straightforwardly from (3.19).

- (i) The Chebyshev polynomials  $T_n(x)$  satisfy the following three-term recurrence relation:

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n = 1, 2, 3, \dots, \quad (3.20)$$

with starting values  $T_0(x) = 1$ ,  $T_1(x) = x$ .



**Figure 3.3.** Chebyshev polynomials of the first kind  $T_n(x)$ ,  $n = 0, 1, 2, 3, 4, 5$ .

Explicit expressions for the first six Chebyshev polynomials are

$$\begin{aligned}
 T_0(x) &= 1, & T_1(x) &= x, \\
 T_2(x) &= 2x^2 - 1, & T_3(x) &= 4x^3 - 3x, \\
 T_4(x) &= 8x^4 - 8x^2 + 1, & T_5(x) &= 16x^5 - 20x^3 + 5x.
 \end{aligned}
 \tag{3.21}$$

The graphs of these Chebyshev polynomials are plotted in Figure 3.3.

- (ii) The leading coefficient (of  $x^n$ ) in  $T_n(x)$  is  $2^{n-1}$  and  $T_n(-x) = (-1)^n T_n(x)$ .
- (iii)  $T_n(x)$  has  $n$  zeros which lie in the interval  $(-1, 1)$ . They are given by

$$x_k = \cos\left(\frac{2k+1}{2n}\pi\right), \quad k = 0, 1, \dots, n-1.
 \tag{3.22}$$

$T_n(x)$  has  $n+1$  extrema in the interval  $[-1, 1]$  and they are given by

$$x'_k = \cos\frac{k\pi}{n}, \quad k = 0, 1, \dots, n.
 \tag{3.23}$$

At these points, the values of the polynomials are  $T_n(x'_k) = (-1)^k$ .

With these properties, it is easy to prove Theorem 3.4, which can also be expressed in the following way.

**Theorem 3.6.** *The polynomial  $\hat{T}_n(x) = 2^{1-n}T_n(x)$  is the minimax approximation on  $[-1, 1]$  to the zero function by a monic polynomial of degree  $n$  and*

$$\|\hat{T}_n\| = 2^{1-n}. \quad (3.24)$$

**Proof.** Let us suppose that there exists a monic polynomial  $p_n$  of degree  $n$  such that  $|p_n(x)| \leq 2^{1-n}$  for all  $x \in [-1, 1]$ , and we will arrive at a contradiction.

Let  $x'_k, k = 0, \dots, n$ , be the abscissas of the extreme values of the Chebyshev polynomial of degree  $n$ . Because of property (ii) of this section we have

$$p_n(x'_0) < 2^{1-n}T_n(x'_0), \quad p_n(x'_1) > 2^{1-n}T_n(x'_1), \quad p_n(x'_2) > 2^{1-n}T_n(x'_2), \dots$$

Therefore, the polynomial

$$Q(x) = p_n(x) - 2^{1-n}T_n(x)$$

changes sign between each two consecutive extrema of  $T_n(x)$ . Thus, it changes sign  $n$  times. But this is not possible because  $Q(x)$  is a polynomial of degree smaller than  $n$  (it is a subtraction of two monic polynomials of degree  $n$ ).  $\square$

**Remark 1.** The monic Chebyshev polynomial  $\hat{T}_n(x)$  is not the minimax approximation in  $\mathbb{P}_n$  (Definition 3.1) of the zero function. The minimax approximation in  $\mathbb{P}_n$  of the zero function is the zero polynomial.

### Further properties

Next we summarize additional properties of the Chebyshev polynomials of the first kind that will be useful later. For further properties and proofs of these results see, for instance, [148, Chaps. 1–2].

#### (a) Relations with derivatives.

$$\begin{cases} T_0(x) = T_1'(x), \\ T_1(x) = \frac{1}{4}T_2'(x), \\ T_n(x) = \frac{1}{2} \left( \frac{T_{n+1}'(x)}{n+1} - \frac{T_{n-1}'(x)}{n-1} \right), \quad n \geq 2, \end{cases} \quad (3.25)$$

$$(1-x^2)T_n'(x) = n[xT_n(x) - T_{n+1}(x)] = n[T_{n-1}(x) - xT_n(x)]. \quad (3.26)$$

#### (b) Multiplication relation.

$$2T_r(x)T_q(x) = T_{r+q}(x) + T_{|r-q|}(x), \quad (3.27)$$

with the particular case  $q = 1$ ,

$$2xT_r(x) = T_{r+1}(x) + T_{|r-1|}(x). \quad (3.28)$$



**(c) Orthogonality relation.**

$$\int_{-1}^1 T_r(x)T_s(x)(1-x^2)^{-1/2} dx = N_r\delta_{rs}, \quad (3.29)$$

with  $N_0 = \pi$  and  $N_r = \frac{1}{2}\pi$  if  $r \neq 0$ .

**(d) Discrete orthogonality relation.**

1. With the zeros of  $T_{n+1}(x)$  as nodes: Let  $n > 0$ ,  $r, s \leq n$ , and let  $x_j = \cos((j + 1/2)\pi/(n + 1))$ . Then

$$\sum_{j=0}^n T_r(x_j)T_s(x_j) = K_r\delta_{rs}, \quad (3.30)$$

where  $K_0 = n + 1$  and  $K_r = \frac{1}{2}(n + 1)$  when  $1 \leq r \leq n$ .

2. With the extrema of  $T_n(x)$  as nodes: Let  $n > 0$ ,  $r, s \leq n$ , and  $x_j = \cos(\pi j/n)$ . Then

$$\sum_{j=0}^n {}''T_r(x_j)T_s(x_j) = K_r\delta_{rs}, \quad (3.31)$$

where  $K_0 = K_n = n$  and  $K_r = \frac{1}{2}n$  when  $1 \leq r \leq n - 1$ .

The double prime indicates that the terms with suffixes  $j = 0$  and  $j = n$  are to be halved.

**(e) Polynomial representation.**

The expression of  $T_n(x)$  in terms of powers of  $x$  is given by (see [38, 201])

$$T_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} d_k^{(n)} x^{n-2k}, \quad (3.32)$$

where

$$d_k^{(n)} = (-1)^k 2^{n-2k-1} \frac{n}{n-k} \binom{n-k}{k}, \quad 2k < n, \quad (3.33)$$

and

$$d_k^{(2k)} = (-1)^k, \quad k \geq 0. \quad (3.34)$$

**(f) Power representation.**

The power  $x^n$  can be expressed in terms of Chebyshev polynomials as follows:

$$x^n = 2^{1-n} \sum_{k=0}^{\lfloor n/2 \rfloor} {}' \binom{n}{k} T_{n-2k}(x), \quad (3.35)$$

where the prime indicates that the term for  $k = 0$  is to be halved.

The first three properties are immediately obtained from the definition of Chebyshev polynomials.

Property (c) means that the set of Chebyshev polynomials  $\{T_n(x)\}$  is an orthogonal set with respect to the weight function  $w(x) = (1 - x^2)^{-1/2}$  in the interval  $(-1, 1)$ . This concept is developed in Chapter 5, and it is shown that this orthogonality implies the first discrete orthogonality of property (d); see (5.86). This property, as well as the second discrete orthogonality, can also be easily proved using trigonometry (see [148, Chap. 4]). See also [148, Chap. 2] for a proof of the last two properties.

### Shifted Chebyshev polynomials

Shifted Chebyshev polynomials are also of interest when the range of the independent variable is  $[0, 1]$  instead of  $[-1, 1]$ . The *shifted Chebyshev polynomials of the first kind* are defined as

$$T_n^*(x) = T_n(2x - 1), \quad 0 \leq x \leq 1. \quad (3.36)$$

Similarly, one can also build shifted polynomials for a generic interval  $[a, b]$ .

Explicit expressions for the first six shifted Chebyshev polynomials are

$$\begin{aligned} T_0^*(x) &= 1, \\ T_1^*(x) &= 2x - 1, \\ T_2^*(x) &= 8x^2 - 8x + 1, \\ T_3^*(x) &= 32x^3 - 48x^2 + 18x - 1, \\ T_4^*(x) &= 128x^4 - 256x^3 + 160x^2 - 32x + 1, \\ T_5^*(x) &= 512x^5 - 1280x^4 + 1120x^3 - 400x^2 + 50x - 1. \end{aligned} \quad (3.37)$$

### 3.3.2 Chebyshev polynomials of the second, third, and fourth kinds

Chebyshev polynomials of the first kind are a particular case of Jacobi polynomials  $P_n^{(\alpha, \beta)}(x)$  (up to a normalization factor). Jacobi polynomials, which can be defined through the Gauss hypergeometric function (see §2.3) as

$$P_n^{(\alpha, \beta)}(x) = \binom{n + \alpha}{n} {}_2F_1 \left( \begin{matrix} -n, n + \alpha + \beta + 1 \\ \alpha + 1 \end{matrix}; \frac{1 - x}{2} \right), \quad (3.38)$$

are orthogonal polynomials on the interval  $[-1, 1]$  with respect to the weight function  $w(x) = (1 - x)^\alpha(1 + x)^\beta$ ,  $\alpha, \beta > -1$ , that is,

$$\int_{-1}^1 P_r^{(\alpha, \beta)}(x) P_s^{(\alpha, \beta)}(x) w(x) dx = M_r \delta_{rs}. \quad (3.39)$$

In particular, for the case  $\alpha = \beta = -1/2$  we recover the orthogonality relation (3.29). Furthermore,

$$T_n(x) = {}_2F_1 \left( \begin{matrix} -n, n \\ 1/2 \end{matrix}; \frac{1 - x}{2} \right). \quad (3.40)$$

As we have seen, an important property satisfied by the polynomials  $T_n(x)$  is that, with the change  $x = \cos \theta$ , the zeros and extrema are equally spaced in the  $\theta$  variable. The zeros of  $T_n(x)$  (see (3.18)) satisfy

$$\theta_k - \theta_{k-1} = |\cos^{-1}(x_k) - \cos^{-1}(x_{k-1})| = \pi/n, \quad (3.41)$$

and similarly for the extrema.

This is not the only case of Jacobi polynomials with equally spaced zeros (in the  $\theta$  variable), but it is the only case with both zeros and extrema equispaced. Indeed, considering the Liouville–Green transformation (see §2.2.4) with the change of variable  $x = \cos \theta$ , we can prove that

$$u_n^{(\alpha,\beta)}(\theta) = \left(\sin \frac{1}{2}\theta\right)^{\alpha+1/2} \left(\cos \frac{1}{2}\theta\right)^{\beta+1/2} P_n^{(\alpha,\beta)}(\cos \theta), \quad 0 \leq \theta \leq \pi, \quad (3.42)$$

satisfies the differential equation

$$\frac{d^2 u_n^{(\alpha,\beta)}(\theta)}{d\theta^2} + \Omega(\theta) u_n^{(\alpha,\beta)}(\theta) = 0, \quad (3.43)$$

$$\Omega(\theta) = \frac{1}{4} \left[ (2n + \alpha + \beta + 1)^2 + \frac{\frac{1}{4} - \alpha^2}{\sin^2 \frac{1}{2}\theta} + \frac{\frac{1}{4} - \beta^2}{\cos^2 \frac{1}{2}\theta} \right].$$

From this, we observe that for the values  $|\alpha| = |\beta| = \frac{1}{2}$ , and only for these values,  $\Omega(\theta)$  is constant and therefore the solutions are trigonometric functions

$$u_n^{(\alpha,\beta)} = C^{(\alpha,\beta)} \cos(\theta w_n^{(\alpha,\beta)} + \phi^{(\alpha,\beta)}), \quad w_n^{(\alpha,\beta)} = n + (\alpha + \beta + 1)/2 \quad (3.44)$$

with  $C^{(\alpha,\beta)}$  and  $\phi^{(\alpha,\beta)}$  values not depending on  $\theta$ . The solutions  $u_n^{(\alpha,\beta)}$ ,  $|\alpha| = |\beta| = \frac{1}{2}$  have therefore equidistant zeros and extrema. The distance between zeros is

$$\theta_k - \theta_{k-1} = \frac{\pi}{n + (\alpha + \beta + 1)/2}. \quad (3.45)$$

Jacobi polynomials have the same zeros as the solutions  $u_n^{(\alpha,\beta)}$  (except that  $\theta = 0, \pi$  may also be zeros for the latter). Therefore, Jacobi polynomials have equidistant zeros for  $|\alpha| = |\beta| = \frac{1}{2}$ . However, due to the sine and cosine factors in (3.42), the extrema of Jacobi polynomials are only equispaced when  $\alpha = \beta = -\frac{1}{2}$ .

The four types of Chebyshev polynomials are the only classical orthogonal (hypergeometric) polynomials for which the elementary change of variables  $x = \cos \theta$  makes all zeros equidistant. Furthermore, these are the only possible cases for which equidistance takes place, not only in the  $\theta$  variable but also under more general changes of variable (also including confluent cases) [52, 53].

Chebyshev polynomials are proportional to the Jacobi polynomials with equispaced  $\theta$  zeros. From (3.42) such Chebyshev polynomials can be written as

$$T_n^{\alpha,\beta}(\theta) = C^{(\alpha,\beta)} \frac{\cos(\theta w_n^{(\alpha,\beta)} + \phi^{(\alpha,\beta)})}{\left(\sin \frac{1}{2}\theta\right)^{\alpha+1/2} \left(\cos \frac{1}{2}\theta\right)^{\beta+1/2}}. \quad (3.46)$$

$C^{(\alpha,\beta)}$  can be arbitrarily chosen and it is customary to take  $C^{(\alpha,\beta)} = 1$ , except when  $\alpha = \beta = \frac{1}{2}$ , in which case  $C^{(\alpha,\beta)} = \frac{1}{2}$ . On the other hand, for each selection of  $\alpha$  and  $\beta$  (with  $|\alpha| = |\beta| = \frac{1}{2}$ ) there is only one possible selection of  $\phi^{(\alpha,\beta)}$  in  $[0, \pi]$  which gives a polynomial solution. This phase is easily selected by requiring that  $T_n^{\alpha,\beta}(\theta)$  be finite as  $\theta \rightarrow 0, \pi$ . With the standard normalization considered, the four families of polynomials  $T_n^{\alpha,\beta}(\theta)$  (proportional to  $P_n^{(\alpha,\beta)}$ ) can be written as

$$\begin{aligned} T_n^{(-1/2,-1/2)}(\theta) &= \cos(n\theta) = T_n(x), \\ T_n^{(1/2,1/2)}(\theta) &= \frac{\sin((n+1)\theta)}{\sin\theta} = U_n(x), \\ T_n^{(-1/2,1/2)}(\theta) &= \frac{\cos((n+\frac{1}{2})\theta)}{\cos(\frac{1}{2}\theta)} = V_n(x), \\ T_n^{(1/2,-1/2)}(\theta) &= \frac{\sin((n+\frac{1}{2})\theta)}{\sin(\frac{1}{2}\theta)} = W_n(x). \end{aligned} \tag{3.47}$$

These are the Chebyshev polynomials of first ( $T$ ), second ( $U$ ), third ( $V$ ), and fourth ( $W$ ) kinds. The third- and fourth-kind polynomials are trivially related because  $P_n^{(\alpha,\beta)}(x) = (-1)^n P_n^{(\beta,\alpha)}(-x)$ .

Particularly useful for some applications are Chebyshev polynomials of the second kind. The zeros of  $U_n(x)$  plus the nodes  $x = -1, 1$  (that is, the  $x$  zeros of  $u_n^{(1/2,1/2)}(\theta(x))$ ) are the nodes of the Clenshaw–Curtis quadrature rule (see §9.6.2). All Chebyshev polynomials satisfy three-term recurrence relations, as is the case for any family of orthogonal polynomials; in particular, the Chebyshev polynomials of the second kind satisfy the same recurrence as the polynomials of the first kind. See [2] or [148] for further properties.

### 3.4 Chebyshev interpolation

Because the scaled Chebyshev polynomial  $\hat{T}_{n+1}(x) = 2^{-n} T_{n+1}(x)$  is the monic polynomial of degree  $n+1$  with the smallest maximum absolute value in  $[-1, 1]$  (Theorem 3.6), the selection of its  $n$  zeros for Lagrange interpolation leads to interpolating polynomials for which the Runge phenomenon is absent.

By considering the estimation for the Lagrange interpolation error (3.6) under the condition of Theorem 3.2, taking as interpolation nodes the zeros of  $T_{n+1}(x)$ ,

$$x_k = \cos\left(\left(k + \frac{1}{2}\right) \frac{\pi}{n+1}\right), \quad k = 0, \dots, n, \tag{3.48}$$

and considering the minimax property of the nodal polynomial  $\hat{T}_{n+1}(x)$  (Theorem 3.6), the following error bound can be obtained:

$$|R_n(x)| = \frac{|f^{(n+1)}(\zeta_x)|}{(n+1)!} |\hat{T}_{n+1}(x)| \leq 2^{-n} \frac{|f^{(n+1)}(\zeta_x)|}{(n+1)!} \leq \frac{1}{2^n (n+1)!} \|f^{(n+1)}\|, \tag{3.49}$$

where  $\|f^{(n+1)}\| = \max_{x \in [-1, 1]} |f^{(n+1)}(x)|$ . By considering a linear change of variables (3.14), an analogous result can be given for Chebyshev interpolation in an interval  $[a, b]$ .

Interpolation with Chebyshev nodes is not as good as the best approximation (Definition 3.1), but usually it is the best practical possibility for interpolation and certainly much better than equispaced interpolation. The best polynomial approximation is characterized by the Chebyshev equioscillation theorem.

**Theorem 3.7 (Chebyshev equioscillation theorem).** *For any continuous function  $f$  in  $[a, b]$ , a unique minimax polynomial approximation in  $\mathbb{P}_n$  (the space of the polynomials of degree  $n$  at most) exists and is uniquely characterized by the alternating or equioscillation property that there are at least  $n + 2$  points at which  $f(x) - P_n(x)$  attains its maximum absolute value, with alternating signs.*

**Proof.** Proofs of this theorem can be found, for instance, in [48, 189].  $\square$

Because the function  $f(x) - P_n(x)$  alternates signs between each two consecutive extrema, it has at least  $n + 1$  zeros; therefore  $P_n$  is a Lagrange interpolating polynomial, interpolating  $f$  at  $n + 1$  points in  $[a, b]$ . The specific location of these points depends on the particular function  $f$ , which makes the computation of best approximations difficult in general.

Chebyshev interpolation by a polynomial in  $\mathbb{P}_n$ , interpolating the function  $f$  at the  $n + 1$  zeros of  $T_{n+1}(x)$ , can be a reasonable approximation and can be computed in an effective and stable way. Given the properties of the error for Chebyshev interpolation on  $[-1, 1]$  and the uniformity in the deviation of Chebyshev polynomials with respect to zero (Theorem 3.6), one can expect that Chebyshev interpolation gives a fair approximation to the minimax approximation when the variation of  $f$  is soft. In addition, the Runge phenomenon does not occur.

Uniform convergence (in the sense of (3.12)) does not necessarily hold but, in fact, there is no system of preassigned nodes that can guarantee uniform convergence for any continuous function  $f$  (see [189, Thm. 4.3]). The sequence of best uniform approximations  $p_n$  for a given continuous function  $f$  does uniformly converge. For the Chebyshev interpolation we need to consider some additional “level of continuity” in the form of the *modulus of continuity*.

**Definition 3.8.** *Let  $f$  be a function defined in an interval  $[a, b]$ . We define the modulus of continuity as*

$$\omega(\delta) = \sup_{\substack{x_1, x_2 \in [a, b] \\ |x_1 - x_2| < \delta}} |f(x_1) - f(x_2)|. \quad (3.50)$$

With this definition, it is easy to see that continuity is equivalent to  $\omega(\delta) \rightarrow 0$  as  $\delta \rightarrow 0$ , while differentiability is equivalent to  $\omega(\delta) = \mathcal{O}(\delta)$ .

**Theorem 3.9 (Jackson’s theorem).** *The sequence of best polynomial approximations  $B_n(f) \in \mathbb{P}_n$  to a function  $f$ , continuous on  $[-1, 1]$ , satisfies*

$$\|f - B_n(f)\| \leq K\omega(1/n), \quad (3.51)$$

*$K$  being a constant.*

**Proof.** For the proof see [189, Chap. 1].  $\square$

This result means that the sequence of best approximations converges uniformly for continuous functions. The situation is not so favorable for Chebyshev interpolation.

**Theorem 3.10.** *Let  $P_n \in \mathbb{P}_n$  be the Chebyshev interpolation polynomial for  $f$  at  $n + 1$  points. Then*

$$\|f - P_n\| \leq M(n), \quad \text{with } M(n) \sim C\omega(1/n) \log n, \quad (3.52)$$

as  $n \rightarrow \infty$ ,  $C$  being a constant.

**Proof.** For the proof see [189, Chap. 4].  $\square$

The previous theorem shows that continuity is not enough and that the condition  $\log(\delta)\omega(\delta) \rightarrow 0$  as  $\delta \rightarrow 0$  is required. This is more demanding than continuity but less demanding than differentiability. When such a condition is satisfied for a function  $f$  it is said that the function is *Dini–Lipschitz continuous*.

### 3.4.1 Computing the Chebyshev interpolation polynomial

Using the orthogonality properties of Chebyshev polynomials, one can compute the Chebyshev interpolation polynomials in an efficient way.

First, we note that, because of the orthogonality relation (3.29), which we abbreviate as  $\langle T_r, T_s \rangle = N_r \delta_{rs}$ , the set  $\{T_k\}_{k=0}^n$  is a set of linearly independent polynomials; therefore,  $\{T_k\}_{k=0}^n$  is a base of the linear vector space  $\mathbb{P}_n$ .

Now, given the polynomial  $P_n \in \mathbb{P}_n$  that interpolates  $f$  at the  $n + 1$  zeros of  $T_{n+1}(x)$ , because  $\{T_k\}_{k=0}^n$  is a base we can write  $P_n$  as a combination of this base, that is,

$$P_n(x) = \sum'_{k=0}^n c_k T_k(x), \quad (3.53)$$

where the prime indicates that the first term is to be halved (which is convenient for obtaining a simple formula for all the coefficients  $c_k$ ). For computing the coefficients, we use the discrete orthogonality relation (3.30). Because  $P_n$  interpolates  $f$  at the  $n + 1$  Chebyshev nodes, we have at these nodes  $f(x_k) = P_n(x_k)$ . Hence,

$$\sum_{j=0}^n f(x_j) T_k(x_j) = \sum'_{i=0}^n c_i \sum_{j=0}^n T_i(x_j) T_k(x_j) = \sum'_{i=0}^n c_i K_i \delta_{ik} = \frac{1}{2}(n+1)c_k. \quad (3.54)$$

Therefore, the coefficients in (3.53) can be computed by means of the formula

$$c_k = \frac{2}{n+1} \sum_{j=0}^n f(x_j) T_k(x_j), \quad x_j = \cos\left(\left(j + \frac{1}{2}\right) \pi / (n+1)\right). \quad (3.55)$$

This type of Chebyshev sum can be efficiently computed in a numerically stable way by means of Clenshaw's method discussed in §3.7. The coefficients can also be written in the form

$$c_k = \frac{2}{n+1} \sum_{j=0}^n f(\cos \theta_j) \cos(k\theta_j), \quad \theta_j = \left(j + \frac{1}{2}\right) \pi / (n+1), \quad (3.56)$$

which, apart from the factor  $2/(n+1)$ , is a discrete cosine transform (named DCT-II or simply DCT) of the vector  $f(\cos \theta_j)$ ,  $j = 0, \dots, n$ .

### Interpolation by orthogonal polynomials

The method used previously for computing interpolation polynomials can be used for building other interpolation formulas. All that is required is that we use a set of orthogonal polynomials  $\{p_n\}$ , satisfying

$$\int_a^b p_n(x) p_m(x) w(x) dx = M_n \delta_{nm}, \quad (3.57)$$

where  $M_n \neq 0$  for all  $n$ , for a suitable weight function  $w(x)$  on  $[a, b]$  (nonnegative and continuous on  $(a, b)$ ) and satisfying a discrete orthogonality relation over the interpolation nodes  $x_k$  of the form

$$\sum_{j=0}^n w_{j,r} p_r(x_j) p_s(x_j) = \delta_{rs}, \quad r, s \leq n. \quad (3.58)$$

When this is satisfied,<sup>1</sup> it is easy to check, by proceeding as before, that the polynomial interpolating a function  $f$  at the nodes  $x_k$ ,  $k = 0, \dots, n$ , can be written as

$$P_n(x) = \sum_{j=0}^n a_j p_j(x), \quad a_j = \sum_{k=0}^n w_{k,j} f(x_k) p_j(x_k). \quad (3.59)$$

In addition, the coefficients can be computed by using a Clenshaw scheme, similar to Algorithm 3.1.

### Chebyshev interpolation of the second kind

For later use, we consider a different type of interpolation, based on the nodes  $x_k = \cos(k\pi/n)$ ,  $k = 0, \dots, n$ . These are the zeros of  $U_{n-1}(x)$  complemented with  $x_0 = 1$ ,  $x_n = -1$  (that is, the zeros of  $u_n^{(1/2, 1/2)}(\cos^{-1} x)$ ; see (3.42)). Also, these zeros are the extrema of  $T_n(x)$ .

We write this interpolation polynomial as

$$P_n(x) = \sum_{k=0}^n c_k T_k(x), \quad (3.60)$$

<sup>1</sup>In Chapter 5, it is shown that this type of relation always exists when the  $x_k$  are chosen to be the zeros of  $p_{n+1}$  and  $w_{k,j} = w_k$  are the weights of the corresponding Gaussian quadrature rule.

and considering the second discrete orthogonality property (3.31), we have

$$c_k = \frac{2}{n} \sum_{j=0}^n f(x_j) T_k(x_j), \quad x_j = \cos(j\pi/n), \quad j = 0, \dots, n. \quad (3.61)$$

This can also be written as

$$c_k = \frac{2}{n} \sum_{j=0}^n f(\cos(j\pi/n)) \cos(kj\pi/n), \quad (3.62)$$

which is a discrete cosine transform (named DCT-I) of the vector  $f(\cos(j\pi/n))$ ,  $j = 0, \dots, n$ .

### 3.5 Expansions in terms of Chebyshev polynomials

Under certain conditions of the interpolated function  $f$  (Dini–Lipschitz continuity), Chebyshev interpolation converges when the number of nodes tends to infinity. This leads to a representation of  $f$  in terms of an infinite series of Chebyshev polynomials.

More generally, considering a set of orthogonal polynomials  $\{p_n\}$  (see (3.57)) and a continuous function in the interval of orthogonality  $[a, b]$ , one can consider series of orthogonal polynomials

$$f(x) = \sum_{k=0}^{\infty} c_k p_k(x). \quad (3.63)$$

Taking into account the orthogonality relation (3.57), we have

$$c_k = \frac{1}{M_k} \int_a^b f(x) p_k(x) w(x) dx. \quad (3.64)$$

Proofs of the convergence for this type of expansion for some classical cases (Legendre, Hermite, Laguerre) can be found in [134]. Apart from continuity and differentiability conditions, it is required that

$$\int_a^b f(x)^2 w(x) dx \quad (3.65)$$

be finite. Expansions of this type are called *generalized Fourier series*. The base functions  $\{p_n\}$  can be polynomials or other suitable orthogonal functions.

Many examples exist of the use of this type of expansion in the solution of problems of mathematical physics (see, for instance, [134]). For the sake of uniform approximation, Chebyshev series based on the Chebyshev polynomials of the first kind are the most useful ones and have faster uniform convergence [5]. For convenience, we write the Chebyshev series as

$$f(x) = \sum_{k=0}^{\infty} c_k T_k(x) = \frac{1}{2} c_0 + \sum_{k=1}^{\infty} c_k T_k(x), \quad -1 \leq x \leq 1. \quad (3.66)$$

With this, and taking into account the orthogonality relation (3.29),

$$c_k = \frac{2}{\pi} \int_{-1}^1 \frac{f(x) T_k(x)}{\sqrt{1-x^2}} dx = \frac{2}{\pi} \int_0^{\pi} f(\cos \theta) \cos(k\theta) d\theta. \quad (3.67)$$



For computing the coefficients, one needs to compute the cosine transform of (3.67). For this purpose, fast algorithms can be used for computing fast cosine transforms. A discretization of (3.67) using the trapezoidal rule (Chapter 5) in  $[0, \pi]$  yields

$$c_k \approx \frac{2}{n} \sum_{j=0}^n f\left(\cos \frac{\pi j}{n}\right) \cos \frac{\pi k j}{n}, \quad (3.68)$$

which is a discrete cosine transform. Notice that, when considering this approximation, and truncating the series at  $k = n$  but halving the last term, we have the interpolation polynomial of the second kind of (3.55).

Another possible discretization of the coefficients  $c_k$  is given by (3.60). With this discretization, and truncating the series at  $k = n$ , we obtain the interpolation polynomial of the first kind of degree  $n$ .

Chebyshev interpolation can be interpreted as an approximation to Chebyshev series (or vice versa), provided that the coefficients decay fast and the discretization is accurate. In other words, Chebyshev series can be a good approximation to near minimax approximations (Chebyshev), which in turn are close to minimax approximations.

On the other hand, provided that the coefficients  $c_k$  decrease in magnitude sufficiently rapidly, the error made by truncating the Chebyshev expansion after the terms  $k = n$ , that is,

$$E_n(x) = \sum_{k=n+1}^{\infty} c_k T_k(x), \quad (3.69)$$

will be given approximately by

$$E_n(x) \approx c_{n+1} T_{n+1}(x), \quad (3.70)$$

that is, the error approximately satisfies the equioscillation property (Theorem 3.7).

How fast the coefficients  $c_k$  decrease depends on continuity and differentiability properties of the function to be expanded. The more regular these are, the faster the coefficients decrease (see the next section).

**Example 3.11 (the Chebyshev expansion of  $\arccos x$ ).** Let us consider the Chebyshev expansion of  $f(x) = \arccos x$ ;  $f(x)$  is continuous in  $[-1, 1]$  but is not differentiable at  $x = \pm 1$ . Observing this, we can expect a noticeable departure from the equioscillation property, as we will see.

For this case, the coefficients can be given in explicit form. From (3.67) we obtain  $c_0 = \pi$  and for  $k \geq 1$ ,

$$\begin{aligned} c_k &= \frac{2}{\pi} \int_0^\pi \theta \cos k\theta \, d\theta \\ &= \frac{2}{\pi} \left\{ \left[ \frac{\theta \sin k\theta}{k} \right]_0^\pi - \int_0^\pi \frac{\sin k\theta}{k} \, d\theta \right\} \\ &= \frac{2}{\pi} \left\{ \left[ \frac{\theta \sin k\theta}{k} + \frac{\cos k\theta}{k^2} \right]_0^\pi \right\} \\ &= \frac{2}{\pi} \frac{(-1)^k - 1}{k^2}, \end{aligned} \quad (3.71)$$

from which it follows that

$$c_{2k} = 0, \quad c_{2k-1} = -\frac{2}{\pi} \frac{2}{(2k-1)^2}. \quad (3.72)$$

We conclude that the resulting Chebyshev expansion of  $f(x) = \arccos x$  is

$$\arccos x = \frac{\pi}{2} T_0(x) - \frac{4}{\pi} \sum_{k=1}^{\infty} \frac{T_{2k-1}(x)}{(2k-1)^2}. \quad (3.73)$$

This corresponds with the Fourier expansion

$$|t| - \frac{\pi}{2} = -\frac{4}{\pi} \sum_{k=1}^{\infty} \frac{\cos(2k-1)t}{(2k-1)^2}, \quad t \in [-\pi, \pi]. \quad (3.74)$$

The absolute error when the series is truncated after the term  $k = 5$  is shown in Figure 3.4. Notice the departure from equioscillation close to the endpoints  $x = \pm 1$ , where the function is not differentiable. ■

In the preceding example the coefficients  $c_k$  of the Chebyshev expansion can be obtained analytically. Unfortunately, this situation represents an exception and numerical methods have to be applied in order to obtain the coefficients  $c_k$  (see §3.6). In a later section we give examples of Chebyshev expansions with explicit coefficients for some special functions (see §3.10).

### 3.5.1 Convergence properties of Chebyshev expansions

The rate of convergence of the series in (3.74) is comparable with that of the series  $\sum_{k=1}^{\infty} 1/k^2$ , which is not very impressive. The bad convergence is caused by the analytic property of this function:  $\arccos x$  is not differentiable at the endpoints  $\pm 1$  of the interval.

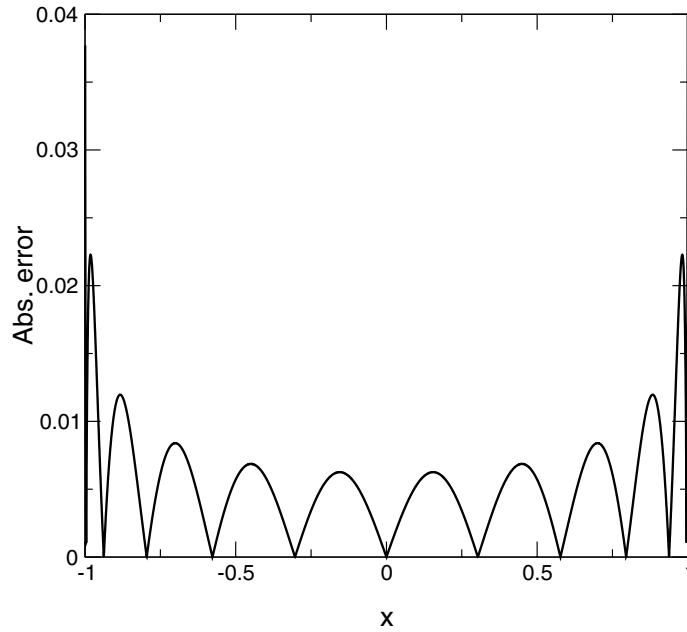
The useful applications of Chebyshev expansions arise when the expansion converges much faster. We give two theorems, the proof of which can be found in [148, §5.7]. We consider expansions of the form (3.66) with partial sum denoted by

$$S_n(x) = \frac{1}{2}c_0 + \sum_{k=1}^n c_k T_k(x). \quad (3.75)$$

**Theorem 3.12 (functions with continuous derivatives).** *When a function  $f$  has  $m + 1$  continuous derivatives on  $[-1, 1]$ , where  $m$  is a finite number, then  $|f(x) - S_n(x)| = \mathcal{O}(n^{-m})$  as  $n \rightarrow \infty$  for all  $x \in [-1, 1]$ .*

**Theorem 3.13 (analytic functions inside an ellipse).** *When a function  $f$  on  $x \in [-1, 1]$  can be extended to a function that is analytic inside an ellipse  $E_r$  defined by*

$$E_r = \left\{ z : \left| z + \sqrt{z^2 - 1} \right| = r \right\}, \quad r > 1, \quad (3.76)$$



**Figure 3.4.** Error after truncating the series in (3.73) after the term  $k = 5$ .

then  $|f(x) - S_n(x)| = \mathcal{O}(r^{-n})$  as  $n \rightarrow \infty$  for all  $x \in [-1, 1]$ .

The ellipse  $E_r$  has semiaxis of length  $(r + 1/r)/2$  on the real  $z$ -axis and of length  $(r - 1/r)/2$  on the imaginary axis.

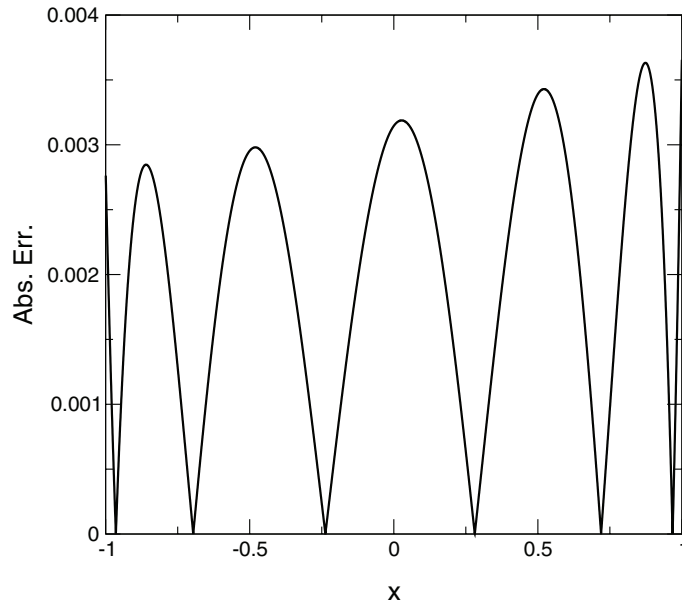
For entire functions  $f$  we can take any number  $r$  in this theorem, and in fact the rate of convergence can be of order  $\mathcal{O}(1/n!)$ . For example, we have the generating function for the modified Bessel coefficients  $I_n(z)$  given by

$$e^{zx} = I_0(z)T_0(x) + 2 \sum_{n=1}^{\infty} I_n(z)T_n(x), \quad -1 \leq x \leq 1, \quad (3.77)$$

where  $z$  can be any complex number. The Bessel functions behave like  $I_n(z) = \mathcal{O}((z/2)^n/n!)$  as  $n \rightarrow \infty$  with  $z$  fixed, and the error  $|e^{zx} - S_n(x)|$  has a similar behavior. The absolute error when the series is truncated after the  $n = 5$  term is shown in Figure 3.5.

### 3.6 Computing the coefficients of a Chebyshev expansion

In general, the Chebyshev coefficients of the Chebyshev expansion of a function  $f$  can be approximately obtained by the numerical computation of the integral of (3.67). To improve the speed of computation, fast Fourier cosine transform algorithms for evaluating the sums in (3.68) can be considered. For numerical aspects of the fast Fourier transform we refer the reader to [226].



**Figure 3.5.** Error after truncating the series for  $e^{2x}$  in (3.77) after the term  $n = 5$ . Compare with Figure 3.4.

In the particular case when the function  $f$  is a solution of an ordinary linear differential equation with polynomial coefficients, Clenshaw [37] proposed an alternative method, which we will now discuss.

### 3.6.1 Clenshaw's method for solutions of linear differential equations with polynomial coefficients

The method works as follows.

Let us assume that  $f$  satisfies a linear differential equation in the variable  $x$  with polynomial coefficients  $p_k(x)$ ,

$$\sum_{k=0}^m p_k(x) f^{(k)}(x) = h(x), \quad (3.78)$$

and where the coefficients of the Chebyshev expansion of the function  $h$  are known. In general, conditions on the solution  $f$  will be given at  $x = 0$  or  $x = \pm 1$ .

Let us express formally the  $s$ th derivative of  $f$  as follows:

$$f^{(s)}(x) = \frac{1}{2}c_0^{(s)} + c_1^{(s)}T_1(x) + c_2^{(s)}T_2(x) + \cdots. \quad (3.79)$$

Then the following expression can be obtained for the coefficients:

$$2rc_r^{(s)} = c_{r-1}^{(s+1)} - c_{r+1}^{(s+1)}, \quad r \geq 1. \quad (3.80)$$

To see how to arrive to this equation, let us start with

$$f'(x) = \frac{1}{2}c_0^{(1)} + c_1^{(1)}T_1(x) + c_2^{(1)}T_2(x) + \cdots + c_{n-1}^{(1)}T_{n-1}(x) \\ + c_n^{(1)}T_n(x) + c_{n+1}^{(1)}T_{n+1}(x) + \cdots \quad (3.81)$$

and integrate this expression. Using the relations in (3.25), we obtain

$$f(x) = \frac{1}{2}c_0 + \frac{1}{2}c_0^{(1)}T_1(x) + \frac{1}{4}c_1^{(1)}T_2(x) + \cdots \\ + \frac{1}{2}c_{n-1}^{(1)}\left(\frac{T_n(x)}{n} - \frac{T_{n-2}(x)}{n-2}\right) \\ + \frac{1}{2}c_n^{(1)}\left(\frac{T_{n+1}(x)}{n+1} - \frac{T_{n-1}(x)}{n-1}\right) \\ + \frac{1}{2}c_{n+1}^{(1)}\left(\frac{T_{n+2}(x)}{n+2} - \frac{T_n(x)}{n}\right) + \cdots \quad (3.82)$$

Comparing the coefficients of the Chebyshev polynomials in this expression and the Chebyshev expansion of  $f$ , we arrive at (3.80) for  $s = 1$ . Observe that a relation for  $c_0$  is not obtained in this way. Substituting in (3.82) given values of  $f$  at, say,  $x = 0$  gives a relation between  $c_0$  and an infinite number of coefficients  $c_n^{(1)}$ .

A next element in Clenshaw's method is using (3.28) to handle the powers of  $x$  occurring in the differential equation satisfied by  $f$ . Denoting the coefficients of  $T_r(x)$  in the expansion of  $g(x)$  by  $C_r(g)$  when  $r > 0$  and twice this coefficient when  $r = 0$ , and using (3.28), we infer that

$$C_r(xf^{(s)}) = \frac{1}{2}\left(c_{r+1}^{(s)} + c_{|r-1|}^{(s)}\right). \quad (3.83)$$

This expression can be generalized as follows:

$$C_r(x^p f^{(s)}) = \frac{1}{2^p} \sum_{j=0}^p \binom{p}{j} c_{|r-p+2j|}^{(s)}. \quad (3.84)$$

When the expansion (3.79) is substituted into the differential equation (3.78) together with (3.80), (3.84), and the associated boundary conditions, it is possible to obtain an infinite set of linear equations for the coefficients  $c_r^{(s)}$ . Two strategies can be used for solving these equations.

**Recurrence method.** The equations can be solved by recurrence for  $r = N - 1, N - 2, \dots, 0$ , where  $N$  is an arbitrary (large) positive integer, by assuming that  $c_r^{(s)} = 0$  for  $r > N$  and by assigning arbitrary values to  $c_N^{(s)}$ . This is done as follows.

Consider  $r = N$  in (3.80) and compute  $c_{N-1}^{(s)}$ ,  $s = 1, \dots, m$ . Then, considering (3.84) and the differential equation (3.78), select  $r$  appropriately in order to compute  $c_{N-1}^{(0)} = c_{N-1}$ . We repeat the process by considering  $r = N - 1$  in (3.80) and computing  $c_{N-2}^{(s)}$ , etc. Obviously and unfortunately, the computed coefficients  $c_r$  will not satisfy, in general, the boundary conditions, and we will have to take care of these in each particular case.

**Iterative method.** The starting point in this case is an initial guess for  $c_r$  which satisfies the boundary conditions. Using these values, we use (3.80) to obtain the values of  $c_r^{(s)}$ ,  $s = 1, \dots, m$ , and then the relation (3.84) and the differential equation (3.78) to compute corrected values of  $c_r$ .

The method based on recursions is, quite often, more rapidly convergent than the iterative method; therefore, and in general, the iterative method could be useful for correcting the rounding errors arising in the application of the method based on recursions.

**Example 3.14 (Clenshaw's method for the  $J$ -Bessel function).** Let us consider, as a simple example (due to Clenshaw), the computation of the Bessel function  $J_0(t)$  in the range  $0 \leq t \leq 4$ . This corresponds to solving the differential equation for  $J_0(4x)$ , that is,

$$xy'' + y' + 16xy = 0 \quad (3.85)$$

in the range  $0 \leq x \leq 1$  with conditions  $y(0) = 1$ ,  $y'(0) = 0$ . This is equivalent to solving the differential equation in  $[-1, 1]$ , because  $J_0(x) = J_0(-x)$ ,  $x \in \mathbb{R}$ .

Because  $J_0(4x)$  is an even function of  $x$ , the  $T_r(x)$  of odd order do not appear in its Chebyshev expansion. By substituting the Chebyshev expansion into the differential equation, we obtain

$$C_r(xy'') + C_r(y') + 16C_r(xy) = 0, \quad r = 1, 3, 5, \dots, \quad (3.86)$$

and considering (3.84),

$$\frac{1}{2}(c''_{r-1} + c''_{r+1}) + c'_r + 8(c_{r-1} + c_{r+1}) = 0, \quad r = 1, 3, 5, \dots \quad (3.87)$$

This equation can be simplified. First, we see that by replacing  $r \rightarrow r - 1$  and  $r \rightarrow r + 1$  in (3.87) and subtracting both expressions, we get

$$\begin{aligned} &\frac{1}{2}(c''_{r-2} + c''_r - c''_r - c''_{r+2}) + (c'_{r-1} - c'_{r+1}) \\ &+ 8(c_{r-2} + c_r - c_r - c_{r+2}) = 0, \quad r = 2, 4, 6, \dots \end{aligned} \quad (3.88)$$

It is convenient to eliminate the terms with the second derivatives. This can be done by using (3.80). In this way,

$$r(c'_{r-1} + c'_{r+1}) + 8(c_{r-2} - c_{r+2}) = 0, \quad r = 2, 4, 6, \dots \quad (3.89)$$

Now, expressions (3.80) and (3.89) can be used alternatively in the recurrence process, as follows:

$$\left. \begin{aligned} c'_{r-1} &= c'_{r+1} + 2rc_r \\ c_{r-2} &= c_{r+2} - \frac{1}{8}r(c'_{r-1} + c'_{r+1}) \end{aligned} \right\} r = N, N - 2, N - 4, \dots, 2. \quad (3.90)$$

As an illustration, let us take as first trial coefficient  $\tilde{c}_{20} = 1$  and all higher order coefficients zero. Applying the recurrences (3.90) and considering the calculation with 15 significant digits, we obtain the values of the trial coefficients given in Table 3.1.

Using the coefficients in Table 3.1, the trial solution of (3.85) at  $x = 0$  is given by

$$\tilde{y}(0) = \frac{1}{2}\tilde{c}_0 - \tilde{c}_2 + \tilde{c}_4 - \tilde{c}_6 + \tilde{c}_8 - \dots = 8050924923505.5, \quad (3.91)$$

**Table 3.1.** *Computed coefficients in the recurrence processes (3.90). We take as starting values  $\tilde{c}_{20} = 1$  and 15 significant digits in the calculations.*

$r$	$\tilde{c}_r$	$\tilde{c}'_{r+1}$
0	807138731281	-8316500240280
2	-5355660492900	13106141731320
4	2004549104041	-2930251101008
6	-267715177744	282331031920
8	18609052225	-15413803680
10	-797949504	545186400
12	23280625	-13548600
14	-492804	249912
16	7921	-3560
18	-100	40
20	1	

**Table 3.2.** *Computed coefficients of the Chebyshev expansion of the solution of (3.85).*

$r$	$c_r$
0	0.1002541619689529 $10^{-0}$
2	-0.6652230077644372 $10^{-0}$
4	0.2489837034982793 $10^{-0}$
6	-0.3325272317002710 $10^{-1}$
8	0.2311417930462743 $10^{-2}$
10	-0.9911277419446611 $10^{-4}$
12	0.2891670860329331 $10^{-5}$
14	-0.6121085523493186 $10^{-7}$
16	0.9838621121498511 $10^{-9}$
18	-0.1242093311639757 $10^{-10}$
20	0.1242093311639757 $10^{-12}$

and the final values for the coefficients  $c_r$  of the solution  $y(x)$  of (3.85) will be obtained by dividing the trial coefficients by  $\tilde{y}(0)$ . This gives the requested values shown in Table 3.2.

The value of  $y(1)$  will then be given by

$$y(1) = \frac{1}{2}c_0 + c_2 + c_4 + c_6 + c_8 + \dots = -0.3971498098638699, \quad (3.92)$$

the relative error being  $0.57 \cdot 10^{-13}$  when compared with the value of  $J_0(4)$ . ■

**Remark 2.** Several questions arise in this successful method. The recursion given in (3.90) is rather simple, and we can find its exact solution; cf. the expansion of the  $J_0$  in (3.139). In Chapter 4 we explain that in this case the backward recursion scheme for computing the Bessel coefficients is stable. In more complicated recursion schemes this information is not available. The scheme may be of large order and may have several solutions of which the asymptotic behavior is unknown. So, in general, we don't know if Clenshaw's method for differential equations computes the solution that we want, and if for the wanted solution the scheme is stable in the backward direction.

**Example 3.15 (Clenshaw's method for the Abramowitz function).** Another but not so easy example of the application of Clenshaw's method is provided by MacLeod [146] for the computation of the Abramowitz functions [1],

$$\mathcal{J}_n(x) = \int_0^\infty t^n e^{-t^2-x/t} dt, \quad n \text{ integer.} \quad (3.93)$$

Chebyshev expansions for  $\mathcal{J}_1(x)$  for  $x \geq 0$  can be obtained by considering the following two cases depending on the range of the argument  $x$ .

If  $0 \leq x \leq a$ ,

$$\mathcal{J}_1(x) = f_1(x) - \sqrt{\pi}xg_1(x) - x^2h_1(x) \log x, \quad (3.94)$$

where  $f_1$ ,  $g_1$ , and  $h_1$  satisfy the system of equations

$$\begin{aligned} xg_1''' + 3g_1'' + 2g_1 &= 0, \\ x^2h_1''' + 6xh_1'' + 6h_1' + 2xh_1 &= 0, \\ xf_1''' + 2f_1 &= 3x^2h_1' + 9xh_1' + 2h_1, \end{aligned} \quad (3.95)$$

with appropriate initial conditions at  $x = 0$ . The functions  $f_1$ ,  $g_1$ , and  $h_1$  are expanded in a series of the form  $\sum_{k=0}^\infty c_k T_k(t)$ , where  $t = (2x^2/a^2) - 1$ .

If  $x > a$ ,

$$\mathcal{J}_1(x) \sim \sqrt{\frac{\pi}{3}} \sqrt{\frac{v}{3}} e^{-v} q_1(v) \quad (3.96)$$

with  $v = 3(x/2)^{2/3}$ . The function  $q_1(v)$  can be expanded in a Chebyshev series of the variable

$$t = \frac{2B}{v} - 1, \quad B = 3 \left( \frac{a}{2} \right)^{2/3}, \quad (3.97)$$

and  $q_1$  satisfies the differential equation

$$4v^3 q_1''' - 12v^3 q_1'' + (12v^3 - 5v)q_1' + (5v + 5)q_1 = 0, \quad (3.98)$$

where the derivatives are taken with respect to  $v$ . The function  $q_1$  is expanded in a series of the form  $\sum_{k=0}^\infty c_k T_k(t)$ , where  $t$  is given in (3.97).

The transition point  $a$  is selected in such a way that  $a$  and  $B$  are exactly represented. Also, the number of terms needed for the evaluation of the Chebyshev expansions for a prescribed accuracy is taken into account.

The differential equations (3.95) and (3.98) are solved by using Clenshaw's method. ■



### 3.7 Evaluation of a Chebyshev sum

Frequently one has to evaluate a partial sum of a Chebyshev expansion, that is, a finite series of the form

$$S_N(x) = \frac{1}{2}c_0 + \sum_{k=1}^N c_k T_k(x). \quad (3.99)$$

Assuming we have already computed the coefficients  $c_k$ ,  $k = 0, \dots, N$ , of the expansion, it would be nice to avoid the explicit computation of the Chebyshev polynomials appearing in (3.99), although they easily follow from the relations (3.18) and (3.19). A first possibility for the computation of this sum is to rewrite the Chebyshev polynomials  $T_k(x)$  in terms of powers of  $x$  and then use the Horner scheme for the evaluation of the resulting polynomial expression. However, one has to be careful when doing this because for some expansions there is a considerable loss of accuracy due to cancellation effects.

#### 3.7.1 Clenshaw's method for the evaluation of a Chebyshev sum

An alternative and efficient method for evaluating this sum is due to Clenshaw [36]. This scheme of computation, which can also be used for computing partial sums involving other types of polynomials, corresponds to the following algorithm.

**ALGORITHM 3.1. Clenshaw's method for a Chebyshev sum.**

*Input:*  $x; c_0, c_1, \dots, c_N$ .

*Output:*  $\tilde{S}_N(x) = \sum_{k=0}^N c_k T_k(x)$ .

- $b_{N+1} = 0; b_N = c_N$ .
- DO  $r = N - 1, N - 2, \dots, 1$ :  

$$b_r = 2xb_{r+1} - b_{r+2} + c_r.$$
- $\tilde{S}_N(x) = xb_1 - b_2 + c_0$ .

Let us explain how we arrived at this algorithm. For simplicity, let us first consider the evaluation of

$$\tilde{S}_N(x) = \sum_{k=0}^N c_k T_k(x) = \frac{1}{2}c_0 + S_N(x). \quad (3.100)$$

This expression can be written in vector form as follows:

$$\tilde{S}_N(x) = \mathbf{c}^T \mathbf{t} = (c_0, c_1, \dots, c_N) \begin{pmatrix} T_0(x) \\ T_1(x) \\ \vdots \\ T_N(x) \end{pmatrix}. \quad (3.101)$$

On the other hand, the three-term recurrence relation satisfied by the Chebyshev polynomials (3.20) can also be written in matrix form,

$$\begin{pmatrix} 1 & & & & & & \\ -2x & 1 & & & & & \\ 1 & -2x & 1 & & & & \\ & 1 & -2x & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & & 1 & -2x & 1 \end{pmatrix} \begin{pmatrix} T_0(x) \\ T_1(x) \\ T_2(x) \\ T_3(x) \\ \vdots \\ T_N(x) \end{pmatrix} = \begin{pmatrix} 1 \\ -x \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad (3.102)$$

or

$$\mathbf{A}\mathbf{t} = \mathbf{d}, \quad (3.103)$$

where  $\mathbf{A}$  is the  $(N + 1) \times (N + 1)$  matrix of the coefficients of the recurrence relation and  $\mathbf{d}$  is the right-hand side vector of (3.102).

Let us now consider a vector  $\mathbf{b}^T = (b_0, b_1, \dots, b_N)$  such that

$$\mathbf{b}^T \mathbf{A} = \mathbf{c}^T. \quad (3.104)$$

Then,

$$\tilde{S}_n = \mathbf{c}^T \mathbf{t} = \mathbf{b}^T \mathbf{A} \mathbf{t} = \mathbf{b}^T \mathbf{d} = b_0 - b_1 x. \quad (3.105)$$

For  $S_N$ , we have

$$S_N = \tilde{S}_N - \frac{1}{2}c_0 = (b_0 - b_1 x) - \frac{1}{2}(b_0 - 2xb_1 + b_2) = \frac{1}{2}(b_0 - b_2). \quad (3.106)$$

The coefficients  $b_r$  can be computed using a recurrence relation if (3.104) is interpreted as the corresponding matrix equation for the recurrence relation (and considering  $b_{N+1} = b_{N+2} = 0$ ). In this way,

$$b_r - 2xb_{r+1} + b_{r+2} = c_r, \quad r = 0, 1, \dots, N. \quad (3.107)$$

The three-term recurrence relation is computed in the backward direction, starting from  $r = N$ . With this, we arrive at

$$\tilde{S}_N = xb_1 - b_2 + c_0, \quad (3.108)$$

$$S_N = xb_1 - b_2 + \frac{c_0}{2}. \quad (3.109)$$

### Error analysis

The expressions provided by (3.105) or (3.106), together with the use of (3.107), are simple and avoid the explicit computation of the Chebyshev polynomials  $T_n(x)$  (with the exception of  $T_0(x) = 1$  and  $T_1(x) = x$ ). However, these relations will be really useful if one can be sure that the influence of error propagation when using (3.107) is small. Let us try to quantify this influence by following the error analysis due to Elliott [62].

Let us denote by

$$\widehat{Q} = Q + \delta Q \quad (3.110)$$

an exact quantity  $Q$  computed approximately ( $\delta Q$  represents the absolute error in the computation).

From (3.107), we obtain

$$\hat{b}_n = \left[ \hat{c}_n + 2x\hat{b}_{n+1} - \hat{b}_{n+2} \right] + r_n, \quad (3.111)$$

where  $r_n$  is the roundoff error arising from rounding the quantity inside the brackets. We can rewrite this expression as

$$\hat{b}_n = \left[ \hat{c}_n + 2x\hat{b}_{n+1} - \hat{b}_{n+2} \right] + \eta_n + r_n, \quad (3.112)$$

where, neglecting the terms of order higher than 1 for the errors,

$$\eta_n = 2(\delta x)\hat{b}_{n+1} \approx 2(\delta x)b_{n+1}. \quad (3.113)$$

From (3.107), it is clear that  $\delta b_n$  satisfies a recurrence relation of the form

$$Y_n - 2xY_{n+1} + Y_{n+2} = \delta c_n + \eta_n + r_n, \quad (3.114)$$

which is the same recurrence relation (with a different right-hand side) as that satisfied by  $b_n$ . It follows that

$$\delta b_0 - \delta b_1 x = \sum_{n=0}^N (\delta c_n + \eta_n + r_n) T_n(x). \quad (3.115)$$

On the other hand, because of (3.105), the computed  $\widetilde{S}_N$  will be given by

$$\widehat{S}_N = \left[ \hat{b}_0 - \hat{b}_1 \hat{x} \right] + s, \quad (3.116)$$

where  $s$  is the roundoff error arising from computing the expression inside the brackets. Hence,

$$\widehat{S}_N = (b_0 - xb_1) + (\delta b_0 - x(\delta b_1)) - b_1(\delta x) + s, \quad (3.117)$$

and using (3.115) it follows that

$$\delta \widehat{S}_N = (\delta b_0 - x\delta b_1) - b_1 \delta x + s = \sum_{n=0}^N (\delta c_n + \eta_n + r_n) T_n(x) - b_1 \delta x + s. \quad (3.118)$$

Let us rewrite this expression as

$$\delta \widehat{S}_N = \sum_{n=0}^N (\delta c_n + r_n) T_n(x) + 2\delta x \sum_{n=0}^N b_{n+1} T_n(x) - b_1 \delta x + s. \quad (3.119)$$

At this point, we can use the fact that the  $b_n$  coefficients can be written in terms of the Chebyshev polynomials of the second kind  $U_n(x)$  as follows:

$$b_n = \sum_{k=n}^N c_k U_{k-n}(x). \quad (3.120)$$

We see that the term  $\sum_{n=0}^N b_{n+1} T_n(x)$  in (3.119) can be expressed as

$$\begin{aligned} \sum_{n=0}^N b_{n+1} T_n(x) &= \sum_{n=1}^N b_n T_{n-1}(x) = \sum_{n=1}^N \left( \sum_{k=n}^N c_k U_{k-n}(x) \right) T_{n-1}(x) \\ &= \sum_{k=1}^N c_k \left( \sum_{n=1}^k U_{k-n}(x) T_{n-1}(x) \right) \\ &= \frac{1}{2} \sum_{k=1}^N c_k (k+1) U_{k-1}(x), \end{aligned} \quad (3.121)$$

where, in the last step, we have used

$$\sum_{n=1}^k \sin(k-n+1)\theta \cos(n-1)\theta = \frac{1}{2}(k+1) \sin k\theta. \quad (3.122)$$

Substituting (3.121) in (3.119) it follows that

$$\delta \tilde{S}_N = \sum_{n=0}^N (\delta c_n + r_n) T_n(x) + \delta x \sum_{n=1}^N n c_n U_{n-1}(x) + s. \quad (3.123)$$

Since  $|T_n(x)| \leq 1$ ,  $|U_{n-1}(x)| \leq n$ , and assuming that the local errors  $|\delta c_n|$ ,  $|r_n|$ ,  $|\delta x|$ ,  $|s|$  are quantities that are smaller than a given  $\epsilon' > 0$ , we have

$$|\delta \tilde{S}_N| \leq \epsilon' \left( (2N+3) + \sum_{n=1}^N n^2 |c_n| \right). \quad (3.124)$$

In the case of a Chebyshev series where the coefficients are slowly convergent, the second term on the right-hand side of (3.124) can provide a significant contribution to the error.

On the other hand, when  $x$  is close to  $\pm 1$ , there is a risk of a growth of rounding errors, and, in this case, a modification of Clenshaw's method [164] seems to be more appropriate. We describe this modification in the following algorithm.

**ALGORITHM 3.2. Modified Clenshaw's method for a Chebyshev sum.**

*Input:*  $x; c_0, c_1, \dots, c_N$ .

*Output:*  $\tilde{S}_N(x) = \sum_{k=0}^N c_k T_k(x)$ .

- IF  $(x \approx \pm 1)$  THEN

- $b_N = c_N; d_N = b_N.$
- IF  $(x \approx 1)$  THEN
  - DO  $r = N - 1, N - 2, \dots, 1:$ 
    - $d_r = 2(x - 1)b_{r+1} + d_{r+1} + c_r.$
    - $b_r = d_r + b_{r+1}.$
- ELSEIF  $(x \approx -1)$  THEN
  - DO  $r = N - 1, N - 2, \dots, 1:$ 
    - $d_r = 2(x + 1)b_{r+1} - d_{r+1} + c_r.$
    - $b_r = d_r - b_{r+1}.$
- ENDIF
- ELSE
  - Use Algorithm 3.1.
- $\tilde{S}_N(x) = xb_1 - b_2 + c_0.$

Oliver [165] has given a detailed analysis of Clenshaw's method for evaluating a Chebyshev sum, also by comparing it with other polynomial evaluation schemes for the evaluation of (3.100); in addition, error bounds are derived. Let us consider two expressions for (3.100),

$$\tilde{S}_N(x) = \sum_{n=0}^N c_n T_n(x), \quad (3.125)$$

$$\tilde{S}_N(x) = \sum_{n=0}^N d_n x^n, \quad (3.126)$$

and let  $\hat{S}_N(x)$  be the actually computed quantity, assuming that errors are introduced at each stage of the computation process of  $\tilde{S}_N(x)$  using (3.125) (considering Clenshaw's method) or (3.126) (considering Horner's scheme). Then,

$$\left| \hat{S}_N(x) - S_N(x) \right| \leq \epsilon \sum_{n=0}^N \rho_n(x) |c_n| \quad (3.127)$$

or

$$\left| \hat{S}_N(x) - S_N(x) \right| \leq \epsilon \sum_{n=0}^N \sigma_n(x) |d_n|, \quad (3.128)$$

depending on the choice of the polynomial expression;  $\epsilon$  is the accuracy parameter and  $\rho_n$  and  $\sigma_n$  are error amplification factors. Reference [165] analyzed the variation of these factors with  $x$ . Two conclusions of this study were that

- the accuracy of the methods of Clenshaw and Horner are sensitive to values of  $x$  and the errors tend to reach their extreme at the endpoints of the interval;
- when a polynomial has coefficients of constant sign or strictly alternating sign, converting into the Chebyshev form does not improve upon the accuracy of the evaluation.

### 3.8 Economization of power series

Chebyshev polynomials also play a key role in the so-called economization of power series. Suppose we have at our disposal a convergent Maclaurin series expansion for the evaluation of a function  $f(x)$  in the interval  $[-1, 1]$ . Then, a plausible approximation to  $f(x)$  may be the polynomial  $p_n(x)$  of degree  $n$ , which is obtained by truncating the power series after  $n + 1$  terms. It may be possible, however, to obtain a “better”  $n$ th-degree polynomial approximation. This is the idea of economization: it involves finding an alternative representation for the function containing  $n + 1$  parameters that possesses the same functional form as the initial approximant. This alternative representation also incorporates information present in the higher orders of the original power series to minimize the maximum error of the new approximant over the range of  $x$ .

Let  $\mathcal{S}_{N+1}$  denote

$$\mathcal{S}_{N+1} = \sum_{i=0}^{N+1} a_i x^i, \quad (3.129)$$

the original Maclaurin series for  $f(x)$  truncated at order  $N + 1$ . Then, one can obtain an “economic” representation by subtracting from  $\mathcal{S}_{N+1}$  a suitable polynomial  $\mathcal{P}_{N+1}$  of the same order such that the leading orders cancel. That is,

$$\mathcal{C}_N = \mathcal{S}_{N+1} - \mathcal{P}_{N+1} = \sum_{i=0}^N a'_i x^i, \quad (3.130)$$

where  $a'_i$  denotes the resulting expansion coefficient of  $x^i$ . Obviously, the idea is to choose  $\mathcal{P}_{N+1}$  in such a way that the maximum error of the new  $N$ th order series representation is significantly reduced. Then, an optimal candidate is

$$\mathcal{P}_{N+1} = a_{N+1} \frac{T_{N+1}}{2^N}. \quad (3.131)$$

The maximum error of this new  $N$ th order polynomial  $\mathcal{C}_N$  is nearly the same as the maximum error of the  $(N + 1)$ th order polynomial  $\mathcal{S}_{N+1}$  and considerably less than  $\mathcal{S}_N$ .

Of course, this procedure may be adapted to ranges different from  $[-1, 1]$  by using Chebyshev polynomials adjusted to the required range. For example, the Chebyshev polynomials  $T_k(x/c)$  (or shifted Chebyshev polynomials  $T_k^*(x/c)$ ) should be used in the range  $[-c, c]$  (or  $[0, c]$ ).

### 3.9 Example: Computation of Airy functions of real variable

The computation of the Airy functions of real variables  $\text{Ai}(x)$ ,  $\text{Bi}(x)$  and their derivatives [186] for real values of the argument  $x$  is a useful example of application of Chebyshev

expansions for computing special functions. As is usual, the real line is divided into a number of intervals and we consider expansions on intervals containing the points  $-\infty$  or  $+\infty$ . An important aspect is selecting the quantity that has to be expanded in terms of Chebyshev polynomials. The Airy functions have oscillatory behavior at  $-\infty$ , and exponential behavior at  $+\infty$ . It is important to expand quantities that are slowly varying in the interval of interest.

When the argument of the Airy function is large, the asymptotic expansions given in (10.4.59)–(10.4.64), (10.4.66), and (10.4.67) of [2] can be considered. The coefficients  $c_k$  and  $d_k$  used in these expansions are given by

$$\begin{aligned} c_0 = 1, \quad c_k &= \frac{\Gamma(3k + \frac{1}{2})}{54^k k! \Gamma(k + \frac{1}{2})}, \quad k = 0, 1, 2, \dots, \\ d_0 = 1, \quad d_k &= -\frac{6k + 1}{6k - 1} c_k, \quad k = 1, 2, 3, \dots \end{aligned} \quad (3.132)$$

#### Asymptotic expansions including the point $-\infty$

We have the representations

$$\begin{aligned} \text{Ai}(-z) &= \pi^{-1/2} z^{-1/4} \left\{ \sin(\zeta + \frac{1}{4}\pi) f(z) - \cos(\zeta + \frac{1}{4}\pi) g(z) \right\}, \\ \text{Ai}''(-z) &= -\pi^{-1/2} z^{1/4} \left\{ \cos(\zeta + \frac{1}{4}\pi) p(z) + \sin(\zeta + \frac{1}{4}\pi) q(z) \right\}, \\ \text{Bi}(-z) &= \pi^{-1/2} z^{-1/4} \left\{ \cos(\zeta + \frac{1}{4}\pi) f(z) + \sin(\zeta + \frac{1}{4}\pi) g(z) \right\}, \\ \text{Bi}'(-z) &= \pi^{-1/2} z^{1/4} \left\{ \sin(\zeta + \frac{1}{4}\pi) p(z) - \cos(\zeta + \frac{1}{4}\pi) q(z) \right\}, \end{aligned} \quad (3.133)$$

where  $\zeta = \frac{2}{3}z^{3/2}$ . The asymptotic expansions for the functions  $f(z)$ ,  $g(z)$ ,  $p(z)$ ,  $q(z)$  are

$$\begin{aligned} f(z) &\sim \sum_{k=0}^{\infty} (-1)^k c_{2k} \zeta^{-2k}, & g(z) &\sim \sum_{k=0}^{\infty} (-1)^k c_{2k+1} \zeta^{-2k-1}, \\ p(z) &\sim \sum_{k=0}^{\infty} (-1)^k d_{2k} \zeta^{-2k}, & q(z) &\sim \sum_{k=0}^{\infty} (-1)^k d_{2k+1} \zeta^{-2k-1}, \end{aligned} \quad (3.134)$$

as  $z \rightarrow \infty$ ,  $|\text{ph } z| < \frac{2}{3}\pi$ .

#### Asymptotic expansions including the point $+\infty$

Now we use the representations

$$\begin{aligned} \text{Ai}(z) &= \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{-\zeta} \tilde{f}(z), & \text{Ai}'(z) &= -\frac{1}{2} \pi^{-1/2} z^{1/4} e^{-\zeta} \tilde{p}(z), \\ \text{Bi}(z) &= \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{\zeta} \tilde{g}(z), & \text{Bi}'(z) &= \frac{1}{2} \pi^{-1/2} z^{1/4} e^{\zeta} \tilde{q}(z), \end{aligned} \quad (3.135)$$

where the asymptotic expansions for the functions  $\tilde{f}(z)$ ,  $\tilde{g}(z)$ ,  $\tilde{p}(z)$ ,  $\tilde{q}(z)$  are

$$\begin{aligned} \tilde{f}(z) &\sim \sum_{k=0}^{\infty} (-1)^k c_k \zeta^{-k}, & \tilde{p}(z) &\sim \sum_{k=0}^{\infty} (-1)^k d_k \zeta^{-k}, \\ \tilde{g}(z) &\sim \sum_{k=0}^{\infty} c_k \zeta^{-k}, & \tilde{q}(z) &\sim \sum_{k=0}^{\infty} d_k \zeta^{-k}, \end{aligned} \quad (3.136)$$

as  $z \rightarrow \infty$ , with  $|\text{ph } z| < \pi$  (for  $\tilde{f}(z)$  and  $\tilde{p}(z)$ ) and  $|\text{ph } z| < \frac{1}{3}\pi$  (for  $\tilde{g}(z)$  and  $\tilde{q}(z)$ ).

### Chebyshev expansions including the point $-\infty$

The functions  $f(z)$ ,  $g(z)$ ,  $p(z)$ ,  $q(z)$  are the slowly varying quantities in the representations in (3.133), and these functions are computed approximately by using Chebyshev expansions. We write  $z = x$ . A possible selection is the  $x$ -interval  $[7, +\infty)$  and for the shifted Chebyshev polynomials we take the argument  $t = (7/x)^3$  (the third power also arises in the expansions in (3.134)). We have to obtain the coefficients in the approximation

$$\begin{aligned} f(x) &\approx \sum_{r=0}^{m_1} a_r T_r^*(t), & g(x) &\approx \frac{1}{\zeta} \sum_{r=0}^{m_2} b_r T_r^*(t), \\ p(x) &\approx \sum_{r=0}^{m_3} c_r T_r^*(t), & q(x) &\approx \frac{1}{\zeta} \sum_{r=0}^{m_4} d_r T_r^*(t). \end{aligned} \quad (3.137)$$

### Chebyshev expansions including the point $+\infty$

Now we consider Chebyshev expansions for the functions  $\tilde{f}(x)$ ,  $\tilde{g}(x)$ ,  $\tilde{p}(x)$ ,  $\tilde{q}(x)$ , and we have

$$\begin{aligned} \tilde{f}(x) &\approx \sum_{r=0}^{n_1} \tilde{a}_r T_r^*(\tilde{t}), & \tilde{g}(x) &\approx \sum_{r=0}^{n_2} (-1)^r \tilde{a}_r T_r^*(\tilde{t}), \\ \tilde{p}(x) &\approx \sum_{r=0}^{n_3} \tilde{c}_r T_r^*(\tilde{t}), & \tilde{q}(x) &\approx \sum_{r=0}^{n_4} (-1)^r \tilde{c}_r T_r^*(\tilde{t}), \end{aligned} \quad (3.138)$$

where  $\tilde{t} = (7/x)^{3/2}$ .

The number of terms in the Chebyshev expansions  $m_j$ ,  $n_j$ ,  $j = 1, 2, 3, 4$ , are determined for a prescribed accuracy of the functions. The Chebyshev coefficients of functions defined by convergent power series can be computed by rearrangement of the corresponding power series expansions using (3.35). For power series that represent asymptotic expansions this method is not available. In the present case we have used the Maple program `chebyshev` with default accuracy of  $10^{-10}$ . The first three coefficients of the Chebyshev expansions (3.137) and (3.138) are given in Table 3.3. For  $\tilde{a}_r$  and  $\tilde{c}_r$ , see Table 3.4 for more—and more precise—values.



**Table 3.3.** *The first coefficients of the Chebyshev expansions (3.137) and (3.138).*

Coef.	$r = 0$	$r = 1$	$r = 2$
$a_r$	1.0001227513	0.0001230753	0.0000003270
$b_r$	0.0695710154	0.0001272386	0.0000006769
$c_r$	0.9998550220	-0.0001453297	-0.0000003548
$d_r$	-0.0973635868	-0.0001420772	-0.0000007225
$\tilde{a}_r$	0.9972733954	-0.0026989587	0.0000271274
$\tilde{c}_r$	1.0038355798	0.0038027377	0.0000322597

### 3.10 Chebyshev expansions with coefficients in terms of special functions

As we have seen in §3.6.1, the coefficients in a Chebyshev expansion can be obtained from recurrence relations when the function satisfies a linear differential equation with polynomial coefficients. All special functions of hypergeometric type satisfy such a differential equation, and in §3.6.1 we have explained how the method works for the Bessel function  $J_0(4x)$  in the range  $-1 \leq x \leq 1$ . However, for this particular function we can obtain expansions in which the coefficients can be expressed in terms of known special functions, which in fact are again Bessel functions. We have (see [143, p. 37])

$$J_0(ax) = \sum_{n=0}^{\infty} \epsilon_n (-1)^n J_n^2(a/2) T_{2n}(x), \quad (3.139)$$

$$J_1(ax) = 2 \sum_{n=0}^{\infty} (-1)^n J_n(a/2) J_{n+1}(a/2) T_{2n+1}(x),$$

where  $-1 \leq x \leq 1$  and  $\epsilon_0 = 1$ ,  $\epsilon_n = 2$  if  $n > 0$ . The parameter  $a$  can be any complex number. Similar expansions are available for  $J$ -Bessel functions of any complex order, in which the coefficients are  ${}_1F_2$ -hypergeometric functions, and explicit recursion relations are available for computing the coefficients. For general integer order, the coefficients are products of two  $J$ -Bessel functions, as in (3.139). See again [143].

Another example is the expansion for the error function,

$$e^{a^2 x^2} \operatorname{erf}(ax) = \sqrt{\pi} e^{\frac{1}{2} a^2} \sum_{n=0}^{\infty} I_{n+\frac{1}{2}} \left( \frac{1}{2} a^2 \right) T_{2n+1}(x), \quad -1 \leq x \leq 1, \quad (3.140)$$

in which the modified Bessel function is used. Again,  $a$  can be any complex number.

The expansions in (3.139) and (3.140) can be viewed as expansions near the origin. Other expansions are available that can be viewed as expansions at infinity, and these may be considered as alternatives for asymptotic expansions of special functions. For example, for the confluent hypergeometric  $U$ -functions we have the convergent expansion in terms of shifted Chebyshev polynomials (see (3.36)):

$$(\omega z)^a U(a, c, \omega z) = \sum_{n=0}^{\infty} C_n(z) T_n^*(1/\omega), \quad z \neq 0, \quad |\operatorname{ph} z| < \frac{3}{2}\pi, \quad 1 \leq \omega \leq \infty. \quad (3.141)$$

Furthermore,  $a, 1 + a - c \neq 0, -1, -2, \dots$ . When equalities hold for these values of  $a$  and  $c$ , the Kummer  $U$ -function reduces to a Laguerre polynomial. This follows from

$$U(a, c, z) = z^{1-c} U(1 + a - c, 2 - c, z) \quad (3.142)$$

and

$$U(-n, \alpha + 1, z) = (-1)^n n! L_n^\alpha(z), \quad n = 0, 1, 2, \dots \quad (3.143)$$

The expansion (3.141) is given in [143, p. 25]. The coefficients can be represented in terms of generalized hypergeometric functions, in fact, Meijer  $G$ -functions, and they can be computed from the recurrence relation

$$\frac{2C_n(z)}{\epsilon_n} = 2(n+1)A_1C_{n+1}(z) + A_2C_{n+2}(z) + A_3C_{n+3}(z), \quad (3.144)$$

where  $b = a + 1 - c$ ,  $\epsilon_0 = \frac{1}{2}$ ,  $\epsilon_n = 1$  ( $n \geq 1$ ), and

$$\begin{aligned} A_1 &= 1 - \frac{(2n+3)(n+a+1)(n+b+1)}{2(n+2)(n+a)(n+b)} - \frac{2z}{(n+a)(n+b)}, \\ A_2 &= 1 - \frac{2(n+1)(2n+3-z)}{(n+a)(n+b)}, \\ A_3 &= -\frac{(n+1)(n+3-a)(n+3-b)}{(n+2)(n+a)(n+b)}. \end{aligned} \quad (3.145)$$

For applying the backward recursion algorithm it is important to know that

$$\sum_{n=0}^{\infty} (-1)^n C_n(z) = 1, \quad |\text{ph } z| < \frac{3}{2}\pi. \quad (3.146)$$

This follows from

$$\lim_{\omega \rightarrow \infty} (\omega z)^a U(a, c, \omega z) = 1 \quad \text{and} \quad T_n^*(0) = (-1)^n. \quad (3.147)$$

The standard backward recursion scheme (see Chapter 4) for computing the coefficients  $C_n(z)$  works only for  $|\text{ph } z| < \pi$ , and for  $\text{ph } z = \pm\pi$  a modification seems to be possible; see [143, p. 26].

Although the expansion in (3.141) converges for all  $z \neq 0$  in the indicated sector, it is better to avoid small values of the argument of the  $U$ -function. Luke gives an estimate of the coefficients  $C_n(z)$  of which the dominant factor that determines the speed of convergence is given by

$$C_n(z) = \mathcal{O}\left(n^{2(2a-c-1)/3} e^{-3n^{2/3}z^{1/3}}\right), \quad n \rightarrow \infty, \quad (3.148)$$

and we see that large values of  $\Re z^{1/3}$  improve the convergence. For example, if we denote  $\zeta = \omega z$  and we want to use the expansion for  $|\zeta| \geq R (> 0)$ , we should choose  $z$  and  $\omega$  ( $\omega \geq 1$ ) such that  $z$  and  $\zeta$  have the same phase, say  $\theta$ . We cannot choose  $z$  with modulus larger than  $R$ , and an appropriate choice is  $z = R e^{i\theta}$ . Then the expansion gives an approximation of the  $U$ -function on the half-ray with  $|\zeta| \geq R$  with phase  $\theta$ , and the coefficients  $C_n(z)$  can be used for all  $\zeta$  on this half-ray. For a single evaluation we can take  $\omega = 1$ .

**Table 3.4.** *Coefficients of the Chebyshev expansion (3.153).*

$n$	$C_n(z)$	$D_n(z)$
0	0.99727 33955 01425	1.00383 55796 57251
1	-0.00269 89587 07030	0.00380 27374 06686
2	0.00002 71274 84648	-0.00003 22598 78104
3	-0.00000 05043 54523	0.00000 05671 25559
4	0.00000 00134 68935	-0.00000 00147 27362
5	-0.00000 00004 63150	0.00000 00004 97977
6	0.00000 00000 19298	-0.00000 00000 20517
7	-0.00000 00000 00938	0.00000 00000 00989
8	0.00000 00000 00052	-0.00000 00000 00054
9	-0.00000 00000 00003	0.00000 00000 00003

The expansion in (3.141) can be used for all special cases of the Kummer  $U$ -function, that is, for Bessel functions (Hankel functions and  $K$ -modified Bessel function), for the incomplete gamma function  $\Gamma(a, z)$ , with special cases the complementary error function and exponential integrals.

**Example 3.16 (Airy function).** For the Airy function  $\text{Ai}(x)$  we have the relations

$$\begin{aligned} \xi^{\frac{1}{6}} U\left(\frac{1}{6}, \frac{1}{3}, \xi\right) &= 2\sqrt{\pi}x^{\frac{1}{4}}e^{\frac{1}{2}\xi}\text{Ai}(x), \\ \xi^{-\frac{1}{6}} U\left(-\frac{1}{6}, -\frac{1}{3}, \xi\right) &= -2\sqrt{\pi}x^{-\frac{1}{4}}e^{\frac{1}{2}\xi}\text{Ai}'(x), \end{aligned} \quad (3.149)$$

where  $\xi = \frac{4}{3}x^{\frac{3}{2}}$ . For the expansions of the functions  $\tilde{f}(x)$  and  $\tilde{p}(x)$  in (3.138) we take  $\omega = (x/7)^{3/2}$  and  $z = \frac{4}{3}7^{3/2} = 24.69\dots$ . To generate the coefficients with this value of  $z$  we determine the smallest value of  $n$  for which the exponential factor in (3.148) is smaller than  $10^{-15}$ . This gives  $n = 8$ .

Next we generate for both  $U$ -functions in (3.149) the coefficients  $C_n(z)$  by using (3.144) in the backward direction, with starting values

$$\tilde{C}_{19}(z) = 1, \quad \tilde{C}_{20}(z) = 0, \quad \tilde{C}_{21}(z) = 0. \quad (3.150)$$

We also compute for normalization

$$S = \sum_{n=0}^{18} (-1)^n \tilde{C}_n(z) = -0.902363242772764 \cdot 10^{25}, \quad (3.151)$$

where the numerical value is for the Ai case. Finally we compute

$$C_n(z) = \tilde{C}_n(z)/S, \quad n = 0, 1, 2, \dots, 9. \quad (3.152)$$

This gives the coefficients  $C_n(z)$  of the expansions

$$\begin{aligned} 2\sqrt{\pi}x^{\frac{1}{4}}e^{\frac{2}{3}x^{3/2}}\text{Ai}(x) &\approx \sum_{n=0}^9 C_n T_n^* \left( (7/x)^{3/2} \right), \\ -2\sqrt{\pi}x^{\frac{1}{4}}e^{\frac{2}{3}x^{3/2}}\text{Ai}'(x) &\approx \sum_{n=0}^9 D_n T_n^* \left( (7/x)^{3/2} \right), \end{aligned} \tag{3.153}$$

$x \geq 7$ , of which the coefficients are given in Table 3.4.

The values of the coefficients in the first three rows of Table 3.4 correspond approximately with the same as those of the coefficients  $\tilde{a}_r$  and  $\tilde{c}_r$  in Table 3.3. ■