SPECIAL FUNCTIONS
AN INTRODUCTION TO THE CLASSICAL FUNCTIONS OF MATHEMATICAL PHYSICS

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Centrum voor Wiskunde en Informatica
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Amsterdam, The Netherlands

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PREFACE

This book gives an introduction to the classical well-known special functions which play a role in mathematical physics, especially in boundary value problems. Usually we call a function "special" when the function, just as the logarithm, the exponential and trigonometric functions (the elementary transcendental functions), belongs to the toolbox of the applied mathematician, the physicist or engineer. Usually there is a particular notation, and a number of properties of the function are known. This branch of mathematics has a respectable history with great names such as Gauss, Euler, Fourier, Legendre, Bessel and Riemann. They all have spent much time on this subject. A great part of their work was inspired by physics and the resulting differential equations. About 70 years ago these activities culminated in the standard work *A Course of Modern Analysis* by Whittaker and Watson, which has had great influence and is still important.

This book has been written with students of mathematics, physics and engineering in mind, and also researchers in these areas who meet special functions in their work, and for whom the results are too scattered in the general literature. Calculus and complex function theory are the basis for all this: integrals, series, residue calculus, contour integration in the complex plane, and so on.

The selection of topics is based on my own preferences, and of course, on what in general is needed for working with special functions in applied mathematics, physics and engineering. This book gives more than a selection of formulas. In the many exercises hints for solutions are often given. In order to keep the book to a modest size, no attention is paid to special functions which are solutions of periodic differential equations such as Mathieu and Lamé functions; these functions are only mentioned when separating the wave equation. The current interest in q-hypergeometric functions would justify an extensive treatment of this topic. It falls outside the scope of the present work, but a short introduction is given nevertheless.

Today students and researchers have computers with formula processors at their disposal. For instance, MATLAB and MATHEMATICA are powerful packages, with possibilities of computing and manipulating special functions. It is very useful to exploit this software, but often extra analysis and knowledge of special functions are needed to obtain optimal results.

At several occasions in the book I have paid attention to the asymptotic and numerical aspects of special functions. When this becomes too specialistic in nature the references to recent literature are given. A separate chapter discusses the stability aspects of recurrence relations for several special functions are discussed. It is explained that a given recursion cannot always be used for computations. Much of this information is available in the literature, but it is difficult for beginners to locate.

Part of the material for this book is collected from well-known books, such as from HOCHSTADT, LEBEDEV, OLVER, RAINVILLE, SZEGÖ and WHITTAKER & WATSON. In addition to these I have used Dutch university lecture notes, in particular those by Prof. H.A. Lauwerier (University of Amsterdam) and Prof. J. Boersma (Technical University Eindhoven).

The enriching and supporting comments of Dick Askey, Johannes Boersma, Tom Koornwinder, Adri Olde Daalhuis, Frank Olver, and Richard Paris on earlier versions of the manuscript are much appreciated. When there are still errors in the many formulas I have myself to blame. But I hope that the extreme standpoint of Dick Askey, who once advised me: *never trust a formula from a book or table; it only gives you an idea how the exact result looks like,* is not applicable to the set of formulas in this book. However, this is a useful warning.

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1

Bernoulli, Euler and Stirling Numbers

A well-known result from calculus is the alternating series

$$\frac{1}{2}\pi = 2\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{2n-1},$$

which can be used for the computation of the number π, although the series converges very slowly. However, summing the first 50 000 terms gives the remarkable result

$$2\sum_{n=1}^{50\,000} \frac{(-1)^{n-1}}{2n-1}$$
$$= 1.5707\ \underline{8}6326\ 79489\ \underline{7}6192\ 31321\ \underline{1}9163\ 975\underline{20\ 5}2098\ 58\underline{331\ 46876}.$$

Using a criterion for convergence of this type of series, we may conclude that this answer is correct to only six significant digits. When you compare the answer on the right-hand side with a 50-d approximation of $\frac{1}{2}\pi$, you will reach the surprising conclusion that nearly all digits in the above approximation are correct, except for those underlined. In this chapter this intriguing aspect will be explained with the help of simple properties of Euler numbers and Boole's summation method. Another example is the series

$$\ln 2 = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n}.$$

You may try to sum the first 50 000 terms with high precision, and compare the answer with an accurate approximation of $\ln 2$.

In this chapter we discuss basic properties of the Bernoulli, Euler and Stirling numbers, with applications to the summation methods of Euler and Boole. These methods are based on the polynomials of Euler and Bernoulli.

Such topics are extensively discussed in classical books on the calculus of differences, the subject that played a prominent part in numerical analysis. A short introduction to difference equations is given §1.1.2.

Just as many other special numbers, polynomials and functions, the special numbers and polynomials of this chapter can be introduced by generating functions. Usually these are power series of the form

$$F(x,t) = \sum_{n=0}^{\infty} f_n(x)t^n,$$

where each f_n is independent of t. The radius of convergence with respect to (complex) values of t may be finite or infinite. We say that $F(x,t)$ is the function which the sequence $\{f_n\}$ generates, and F is called the *generating function*. Often, F and the coefficients f_n are analytic functions in a certain domain.

1.1. Bernoulli Numbers and Polynomials

The Bernoulli numbers are named after Jakob Bernoulli, who mentioned the numbers in his posthumous *Ars conjectandi* of 1713; see BERNOULLI (1713). He discussed *summae potestatum*, sums of equal powers of the first n integers. For instance, we know from elementary calculus that

$$\begin{aligned}
\sum_{i=1}^{n-1} i &= \frac{1}{2}n(n-1) = \frac{1}{2}n^2 - \frac{1}{2}n,\\
\sum_{i=1}^{n-1} i^2 &= \frac{1}{3}n^3 - \frac{1}{2}n^2 + \frac{1}{6}n,\\
\sum_{i=1}^{n-1} i^3 &= \frac{1}{4}n^4 - \frac{1}{2}n^3 + \frac{1}{4}n^2,\\
\sum_{i=1}^{n-1} i^4 &= \frac{1}{5}n^5 - \frac{1}{2}n^4 + \frac{1}{3}n^3 - \frac{1}{30}n,
\end{aligned}$$

and so on. Bernoulli was, in particular, interested in the numbers multiplying the linear terms n at the right-hand sides: $-\frac{1}{2}, \frac{1}{6}, 0, -\frac{1}{30}, \ldots$. EULER (1755) called them Bernoulli numbers $B_1, B_2, B_3, B_4, \ldots$. As we know from the general result

$$\sum_{i=0}^{n-1} i^p = \frac{1}{p+1}\sum_{k=0}^{p}\binom{p+1}{k}B_k n^{p+1-k},$$

they show up in other terms also; see Exercise 1.3.

The Bernoulli numbers occur in practically every field of mathematics, in particular, in combinatorial theory, finite difference calculus, numerical analysis, analytical number theory, and probability theory. We discuss their role in the summation formula of Euler.

1.1.1. Definitions and Properties

Instead of introducing the *Bernoulli numbers* B_n as above, we use a generating function for their definition:

$$\boxed{\frac{z}{e^z-1}=\sum_{n=0}^{\infty}\frac{B_n}{n!}z^n,\quad |z|<2\pi.} \tag{1.1}$$

Because the function

$$f(z)=\frac{z}{e^z-1}-1+\frac{1}{2}z$$

is even (prove it!), all Bernoulli numbers with odd index ≥ 3 vanish:

$$B_{2n+1}=0,\quad n=1,2,3,\ldots\,.$$

The first nonvanishing numbers are

$$B_0=1,\quad B_1=-\frac{1}{2},\quad B_2=\frac{1}{6},\quad B_4=-\frac{1}{30},\quad B_6=\frac{1}{42},$$

$$B_8=-\frac{1}{30},\quad B_{10}=\frac{5}{66},\quad B_{12}=-\frac{691}{2730},\quad B_{14}=\frac{7}{6},\quad B_{16}=-\frac{3617}{510}$$

The *Bernoulli polynomials* are defined by the generating function

$$\boxed{\frac{ze^{xz}}{e^z-1}=\sum_{n=0}^{\infty}\frac{B_n(x)}{n!}z^n,\quad |z|<2\pi.} \tag{1.2}$$

The first few polynomials are

$$\begin{aligned}
B_0(x)&=1,\\
B_1(x)&=x-\frac{1}{2},\\
B_2(x)&=x^2-x+\frac{1}{6},\\
B_3(x)&=x^3-\frac{3}{2}x^2+\frac{1}{2}x,\\
B_4(x)&=x^4-2x^3+x^2-\frac{1}{30}.
\end{aligned}$$

A further step yields the *generalized Bernoulli polynomials*:

$$e^{xz}\left(\frac{z}{e^z-1}\right)^{\sigma}=\sum_{n=0}^{\infty}\frac{B_n^{(\sigma)}(x)}{n!}z^n,\quad |z|<2\pi, \tag{1.3}$$

where σ is any complex number. By taking $x=0$ we obtain the *generalized Bernoulli numbers* $B_n^{(\sigma)}=B_n^{(\sigma)}(0)$, which are polynomials of degree n of the complex variable σ.

We now give some relations which easily follow from the definitions through the generating functions.

$$\int_0^1 B_n(x)\,dx=0,\quad n=1,2,3,\ldots. \tag{1.4}$$

$$B_n(x)=\sum_{k=0}^{n}\binom{n}{k}B_kx^{n-k},\quad B_n(x+y)=\sum_{k=0}^{n}\binom{n}{k}B_k(x)y^{n-k}. \tag{1.5}$$

$$B_n(0)=B_n,\quad B_n(1)=(-1)^nB_n. \tag{1.6}$$

$$B_n(1-x)=(-1)^nB_n(x),\quad B_n(-x)=(-1)^n\left[B_n(x)+nx^{n-1}\right]. \tag{1.7}$$

$$B_n(\tfrac{1}{2})=-\left(1-2^{1-n}\right)B_n. \tag{1.8}$$

$$\frac{d}{dx}B_n(x)=nB_{n-1}(x),\quad B_n(x+1)-B_n(x)=nx^{n-1}. \tag{1.9}$$

$$\sum_{k=0}^{n}\binom{n+1}{k}B_k(x)=(n+1)x^n. \tag{1.10}$$

The proof of (1.4) follows for example by integrating the left-hand side of (1.2) with respect to x. The properties (1.5)–(1.10) all hold for $n=0,1,2,\ldots$. Property (1.10) gives for $x=0$ the identity for the Bernoulli numbers:

$$\sum_{k=0}^{n}\binom{n+1}{k}B_k=0, \tag{1.11}$$

with which the numbers can be generated by means of a simple recursion. Symbolic manipulation on the computer may be very useful here. Numerical computations with finite precision will yield very inaccurate results, due to instability of (1.11).

In Exercise 1.1c you can prove that

$$\tan z=\sum_{n=0}^{\infty}(-1)^{n+1}\frac{T_{2n+1}z^{2n+1}}{(2n+1)!}, \tag{1.12}$$

where the relation between the *tangent numbers* T_n and the Bernoulli numbers B_n is defined by

$$B_n = \frac{-nT_{n-1}}{2^n(2^n-1)}, \quad n = 1, 2, \ldots .$$

T_n is an integer with $T_{2n} = 0$, $n > 0$. This follows from differentiating $\tan z$: all even derivatives at $z = 0$ vanish and the odd derivatives are integers. The same holds for the coefficients of the MacLaurin expansion. We have

$$T_0 = 1, \quad T_1 = -1, \quad T_3 = 2, \quad T_5 = -16, \quad T_7 = 272, \quad T_9 = -7936.$$

Finally, we mention

$$\int_a^x B_n(t)\, dt = \frac{1}{n+1}\left[B_{n+1}(x) - B_{n+1}(a)\right].$$

This property can be used in the proof of the memorable formulas

$$\boxed{\begin{aligned} B_{2n-1}(x) &= 2(-1)^{n+1}(2n-1)! \sum_{m=1}^{\infty} \frac{\sin(2\pi m x)}{(2\pi m)^{2n-1}}, \\ B_{2n}(x) &= 2(-1)^{n+1}(2n)! \sum_{m=1}^{\infty} \frac{\cos(2\pi m x)}{(2\pi m)^{2n}}, \end{aligned}} \tag{1.13}$$

where $n = 1, 2, 3, \ldots$ and $0 \le x \le 1$. For a proof we may begin with the first line with $n = 1$. This gives a well-known result from the theory of Fourier series for the function $B_1(x) = x - \frac{1}{2}$. Then induction and the above integral relation should be used. The special case $x = 0$ gives in (1.5) an interesting result for the even Bernoulli numbers:

$$\boxed{B_{2n} = 2(-1)^{n+1}(2n)! \sum_{m=1}^{\infty} (2\pi m)^{-2n}, \quad n = 1, 2, 3, \ldots .} \tag{1.14}$$

It is of interest, since with this result the series $\sum_{m=1}^{\infty} m^{-s}$ (the Riemann zeta function, which will be discussed in the following chapter) can be expressed in terms of Bernoulli numbers when s is an even positive integer. When $s = 2, 4, 6$ we thus have

$$\begin{aligned} \sum_{m=1}^{\infty} \frac{1}{m^2} &= \frac{\pi^2}{6}, \\ \sum_{m=1}^{\infty} \frac{1}{m^4} &= \frac{\pi^4}{90}, \\ \sum_{m=1}^{\infty} \frac{1}{m^6} &= \frac{\pi^6}{945}. \end{aligned} \tag{1.15}$$

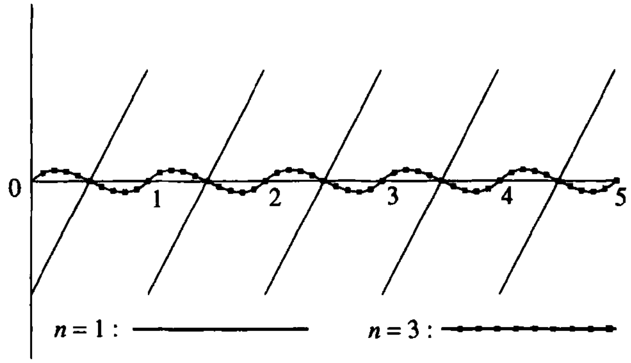

Figure 1.1. The functions $\widetilde{B}_n(x)$, $n = 1$ and $n = 3$.

For odd s−values a similar relation is never found.

The Fourier series for Bernoulli polynomials in (1.13) can be defined for all real values of x. Outside the interval $[0, 1]$ the series do not represent polynomials, of course, but periodic functions of x. These periodic functions are very important, and we introduce a special notation $\widetilde{B}_n(x)$ by defining for $n = 0, 1, 2, \ldots$

$$\widetilde{B}_n(x) = B_n(x), \quad 0 \le x < 1,$$

and

$$\widetilde{B}_n(x+1) = \widetilde{B}_n(x), \quad x \in \mathbb{R}. \tag{1.16}$$

The functions $\widetilde{B}_n(x)$ have continuous derivatives up to order $n-1$. This easily follows from the earlier properties, for instance from (1.13). They become smoother as n increases. As will follow from §1.1.3, the periodic functions $\widetilde{B}_n(x)$ play an important part in *Euler's summation formula*.

In Figures 1.1 and 1.2 we show the first four functions $\widetilde{B}_n(x), n = 1, 2, 3, 4$.

1.1.2. A Simple Difference Equation

One of the results of the previous subsection (see (1.9)) reads

$$f(x+1) - f(x) = nx^{n-1},$$

a *difference equation* with solution $f(x) = B_n(x)$. It follows that the Bernoulli polynomials can be used to construct a solution of the difference equation

$$f(x+1) - f(x) = P_n(x),$$

where $P_n(x)$ is a polynomial. When $P_n(x) = \sum_{k=0}^{n} a_k x^k$, we can write the general solution in the form

$$f(x) = \sum_{k=0}^{n} \frac{a_k}{k+1} B_{k+1}(x) + \pi(x),$$

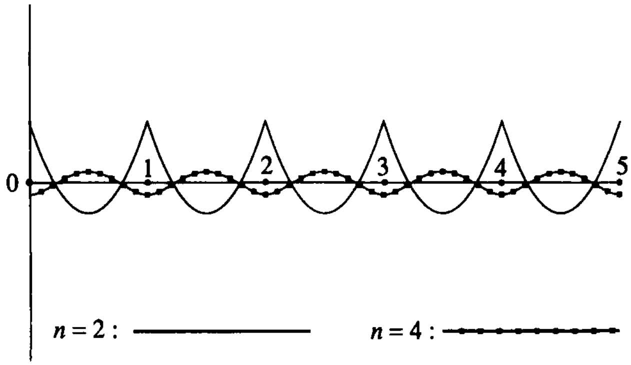

Figure 1.2. The functions $\widetilde{B}_n(x)$, $n = 2$ and $n = 4$.

where $\pi(x)$ is an arbitrary periodic function of x of period 1.

The function $f(x) = \omega^n B_n(\frac{x}{\omega})$ is a solution of the more general difference equation

$$\frac{f(x+\omega) - f(x)}{\omega} = \phi(x), \tag{1.17}$$

with $\phi(x) = nx^{n-1}$. When we want to solve this equation for general $\phi(x)$, we may call

$$f(x) = A - \omega \sum_{n=0}^{\infty} \phi(x + n\omega)$$

a formal solution of the difference equation (1.17), where A is independent of x. For example, when $\phi(x) = \exp(-x)$, we obtain

$$f(x) = A - \omega \sum_{n=0}^{\infty} e^{-x-n\omega} = A - \frac{\omega e^{-x}}{1 - e^{-\omega}},$$

which indeed is a solution of (1.17). The series in this example is convergent, but in general this condition is not satisfied. Several methods are available to use a modified form of the formal solution, from which well-defined solutions can be obtained. For instance, we can take $A = \int_c^N \phi(x)\, dx$, with $c \geq 0$ and N a large integer, and we define

$$f_N(x) = \int_c^N \phi(x)\, dx - \sum_{n=0}^{N} \phi(x + n\omega).$$

When the limit of $f_N(x)$ exists as $N \to \infty$, this limit may be a solution. For example, let $c = 1, \omega = 1$ and $\phi(x) = 1/x,\ x > 0$. Then

$$f_N(x) = \left[\ln N - \sum_{n=0}^{N} \frac{1}{n+1}\right] + \left[\sum_{n=0}^{N} \left(\frac{1}{n+1} - \frac{1}{x+n}\right)\right],$$

and each quantity between square brackets tends to a finite limit, as $N \to \infty$; see the next subsection, Example 1.2. From Chapter 3, formula (3.10), we infer that the function $f_N(x)$ tends to a special function, the logarithmic derivative of the gamma function $\psi(x)$, which indeed satisfies the difference equation $f(x+1) - f(x) = 1/x$.

In a second method the function $\phi(x)$ in (1.17) is replaced with $\phi(x,\mu)$ that satisfies $\lim_{\mu\to 0}\phi(x,\mu) = \phi(x)$. For instance, we can take

$$\phi(x,\mu) = \phi(x)e^{-\mu x}, \quad \mu > 0.$$

Let c be a number independent of x, and assume that

$$\int_c^\infty \phi(x,\mu)\,dx, \quad \text{and} \quad \sum_{n=0}^\infty \phi(x+n\omega,\mu)$$

both converge. Then we define as the solution of (1.17) the function $f(x) = \lim_{\mu\to 0} f(x,\mu)$, where

$$f(x,\mu)) = \left[\int_c^\infty \phi(x,\mu)\,dx - \sum_{n=0}^\infty \phi(x+n\omega,\mu)\right], \tag{1.18}$$

provided that this limit exists. It is shown in the classical literature (for instance, in NÖRLUND (1924)) that this $f(x)$ indeed satisfies (1.17), and that this solution is independent of the particular choice of $\phi(x,\mu)$. Other choices are also possible. It is easily verified that for (1.17) with $c = 1, \omega = 1, \phi(x) = 1$, the function $f(x,\mu)$ is given by

$$f(x,\mu) = \frac{e^{-\mu}}{\mu} - \frac{e^{-\mu x}}{1-e^{-\mu}},$$

and that $\lim_{\mu\to 0} f(x,\mu) = x - \frac{1}{2} = B_1(x)$, a Bernoulli polynomial.

Example 1.1. Consider the difference equation

$$f(x+1) - f(x) = nx^{n-1}e^{-\mu x}, \quad \mu > 0, \quad x > 0,$$

which for $\mu = 0$ reduces to the difference equation of the Bernoulli polynomials. We try to find $f(x,\mu)$ of (1.18). Take $c = 0$, then

$$\begin{aligned} f(x,\mu) &= \int_0^\infty n\,t^{n-1}e^{-\mu t}\,dt - \sum_{m=0}^{\infty} n\,(x+m)^{n-1}e^{-\mu(x+m)} \\ &= n\,(-1)^{n-1}\frac{\partial^{n-1}}{\partial\mu^{n-1}}\left[\int_0^\infty e^{-\mu t}\,dt - \sum_{m=0}^{\infty} e^{-\mu(x+m)}\right] \\ &= n\,(-1)^{n-1}\frac{\partial^{n-1}}{\partial\mu^{n-1}}\left[\frac{1}{\mu} + \frac{e^{-\mu x}}{e^{-\mu}-1}\right] \\ &= n\,(-1)^{n-1}\frac{\partial^{n-1}}{\partial\mu^{n-1}}\left[\sum_{m=1}^{\infty}(-\mu)^{m-1}\frac{B_m(x)}{m!}\right] \\ &= n\sum_{m=n}^{\infty}\frac{(-\mu)^{m-n}B_m(x)}{m\,(m-n)!}. \end{aligned}$$

In this derivation we have used the generating function (1.2). When $\mu \to 0$, we have $f(x,\mu) = B_n(x)$, which again shows that $B_n(x)$ satisfies the second relation in (1.9).

1.1.3. Euler's Summation Formula

A striking application of Bernoulli numbers and polynomials is *Euler's summation formula*, that links a finite or infinite series and an integral. This formula yields an efficient method for evaluating some slowly convergent series by means of an integral. Turning it round, by this method also an integral can be approximated by discretization, which leads to the trapezoidal rule. In EULER (1732) the proof of the formula can be found.

Theorem 1.1. *Let the function f: $[0,1] \to \mathbb{C}$ have k continuous derivatives $(k = 0,1,2,\ldots)$. Then for $k \ge 1$*

$$f(1) = \int_0^1 f(x)\,dx + \sum_{i=1}^{k}\frac{(-1)^iB_i}{i!}\left[f^{(i-1)}(1) - f^{(i-1)}(0)\right] + R_k,$$

with

$$R_k = \frac{(-1)^{k+1}}{k!}\int_0^1 f^{(k)}(x)B_k(x)\,dx.$$

Proof. The proof runs with induction with respect to k. For $k = 1$ the claim is true, which follows from integrating by parts. Then the property

$$B_m(x) = \frac{1}{m+1}B'_{m+1}(x)$$

is used to go from $k = m \ge 1$ to $k = m+1$. ∎

With similar conditions for f on the interval $[j-1, j]$ we have

$$f(j) = \int_{j-1}^{j} f(x)\,dx + \sum_{i=1}^{k} \frac{(-1)^i B_i}{i!} \left[f^{(i-1)}(j) - f^{(i-1)}(j-1) \right] + R_k,$$

with

$$R_k = \frac{(-1)^{k+1}}{k!} \int_{j-1}^{j} f^{(k)}(x) \widetilde{B}_k(x)\,dx,$$

where $\widetilde{B}_k(x)$ is the function introduced in (1.16).

The next step joins a number of these intervals:

$$\sum_{i=1}^{n} f(i) = \int_0^n f(x)\,dx + \sum_{i=1}^{k} \frac{(-1)^i B_i}{i!} \left[f^{(i-1)}(n) - f^{(i-1)}(0) \right] + R_k,$$

with

$$R_k = \frac{(-1)^{k+1}}{k!} \int_0^n f^{(k)}(x) \widetilde{B}_k(x)\,dx.$$

For $k = 1$ this gives the formula

$$f(1) + f(2) + \cdots + f(n) = \int_0^n f(x)\,dx + \tfrac{1}{2}[f(n) - f(0)] + \int_0^n \widetilde{B}_1(x) f'(x)\,dx,$$

with $\widetilde{B}_1(x)$ a sawtooth function on $[0, n]$. This is *Euler's summation formula* in its simplest form. The formula expresses a connection between the sum of the first n terms of a series and the integral of the corresponding function over the interval $[0, n]$.

Example 1.2. Take

$$f(x) = \frac{1}{x+1}$$

and replace in the above formula n with $n - 1$. Then we obtain the classical example

$$1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \cdots + \frac{1}{n} = \ln n + \frac{1}{2n} + \frac{1}{2} - \int_0^{n-1} \widetilde{B}_1(x) \frac{dx}{(1+x)^2}.$$

The integral is convergent when $n \to \infty$. From this we infer that

$$\gamma = \lim_{n\to\infty} \left(1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \cdots + \frac{1}{n} - \ln n \right)$$

exists as well. The limit $\gamma = 0.5772\ 15664\ 90153...$ is called *Euler's constant.* From this example also follows that

$$\gamma = \frac{1}{2} - \int_0^{\infty} \widetilde{B}_1(x) \frac{dx}{(1+x)^2} = \frac{1}{2} - \int_1^{\infty} \widetilde{B}_1(x) \frac{dx}{x^2}.$$

Since

$$B_k(0) = 0, \quad k = 3, 5, 7, \ldots$$

all terms with odd index can be deleted in the summation formula, except the term with index $i = 1$. And at both sides we can add the term $f(0)$. Then the result is

Theorem 1.2. *Let the function f: $[0, n] \to \mathbb{C}$ have $(2k+1)$ continuous derivatives $(k \geq 0, n \geq 1)$. Then*

$$\begin{aligned}\sum_{i=0}^{n} f(i) = \int_0^n f(x)\,dx + \frac{1}{2}[f(n) + f(0)] \\ + \sum_{i=1}^{k} \frac{B_{2i}}{(2i)!}\left[f^{(2i-1)}(n) - f^{(2i-1)}(0)\right] + R_k,\end{aligned} \tag{1.19}$$

with

$$R_k = \frac{1}{(2k+1)!}\int_0^n f^{(2k+1)}(x)\widetilde{B}_{2k+1}(x)\,dx.$$

The summation formula is usually presented in this form, and is connected with the *trapezoidal rule* (Exercise 1.7).

Example 1.3. We take $f(x) = x^2$. Since $f^{(3)}(x) = 0$ for each x, the contribution of the remainder R_k in (1.19) is zero when $k \geq 1$. For $k = 1$ (1.19) then reads

$$\sum_{i=0}^{n} i^2 = \int_0^n x^2\,dx + \frac{1}{2}n^2 + \frac{1}{2}B_2[f'(n) - f'(0)] = \frac{1}{3}n^3 + \frac{1}{2}n^2 + \frac{1}{6}n.$$

An alternative summation formula for infinite series arises through the intermediate form

$$\begin{aligned}\sum_{i=m}^{n} f(i) = \int_m^n f(x)\,dx + \frac{1}{2}[f(n) + f(m)] \\ + \sum_{i=1}^{k} \frac{B_{2i}}{(2i)!}\left[f^{(2i-1)}(n) - f^{(2i-1)}(m)\right] + R_k,\end{aligned} \tag{1.20}$$

with

$$R_k = \frac{1}{(2k+1)!}\int_m^n f^{(2k+1)}(x)\widetilde{B}_{2k+1}(x)\,dx.$$

In this formula we replace n with ∞, which is allowed when the infinite series and the indefinite integrals

$$\sum_{i=m}^{\infty} f(i), \quad \int_m^{\infty} f(x)\,dx, \quad \int_m^{\infty} f^{(2k+1)}(x)\widetilde{B}_{2k+1}(x)\,dx$$

exist. In addition we assume that f and the derivatives occurring in the formula tend to zero when their arguments tend to infinity. The result is

$$\sum_{i=m}^{\infty} f(i) = \int_m^{\infty} f(x)\,dx + \tfrac{1}{2}f(m) - \sum_{i=1}^{k} \frac{B_{2i}}{(2i)!} f^{(2i-1)}(m) + R_k, \tag{1.21}$$

with

$$R_k = \frac{1}{(2k+1)!}\int_m^{\infty} f^{(2k+1)}(x)\widetilde{B}_{2k+1}(x)\,dx.$$

This form of Euler's summation formula can be fruitfully applied in summing infinite series. It is important to have information on the remainder R_k. It is not always necessary to know the integral in R_k exactly. Also, it is not necessary to know whether

$$\lim_{k\to\infty} R_k = 0.$$

In many cases this condition is not fulfilled, or the limit does not even exist. An estimate of the remainder can be obtained through the following theorem.

Theorem 1.3. *Let f and all its derivatives be defined on the interval $[0,\infty)$ on which they should be monotonic and tend to zero when $x \to \infty$. Then R_k of (1.19) satisfies*

$$R_k = \theta_k \frac{B_{2k+2}}{(2k+2)!}\left[f^{(2k+1)}(n) - f^{(2k+1)}(0)\right], \quad \textit{with} \quad 0 \le \theta_k \le 1.$$

Proof. First we remark that

$$f^{(k)}(x), \quad f^{(k+1)}(x), \quad k = 0, 1, 2, \ldots$$

have fixed and different signs on $[0,\infty)$. Let $f(x) > 0$, $x \ge 0$. Then it is easily verified (consider the graph of the sine function) that the sign of

$$\int_0^1 \sin(2\pi m x) f(x)\,dx, \quad m = 1, 2, 3, \ldots$$

is also positive. From (1.13) and (1.16) then follows that the sign of

$$\int_0^n \widetilde{B}_{2n+1}(x) f(x)\,dx, \quad n = 1, 2, 3, \ldots, \quad m = 0, 1, 2, \ldots$$

equals the sign of $(-1)^{n+1}$. From this we also conclude that the remainder R_k of (1.19) have different signs for subsequent values of k. This implies that R_k and $(R_k - R_{k+1})$ have the same sign and hence that

$$|R_k| \leq |R_k - R_{k+1}|.$$

From (1.19) it follows, however, that

$$R_k - R_{k+1} = \frac{B_{2k+2}}{(2k+2)!}\left[f^{(2k+1)}(n) - f^{(2k+1)}(0)\right].$$

This is exactly the 'first neglected term' in Euler's summation formula. The sign of this term equals the sign of R_k and the absolute value of this term at least equals the absolute value of R_k. ■

A similar result holds for formula (1.21). In this case we have

$$R_k = -\theta_k \frac{B_{2k+2}}{(2k+2)!} f^{(2k+1)}(m), \quad \text{with} \quad 0 \leq \theta_k \leq 1. \tag{1.22}$$

The theorem says that, with the conditions on f, the error in taking in (1.21) k terms of the series in the right-hand side is smaller than the first neglected $(k+1)$–th term. In practical problems one tries to find this $(k+1)$–th term that falls below the requested accuracy, and one sums the series on the right-hand side of (1.21) as far as the k–th term. In other words, one may sum the series until a particular term falls below the accuracy. This naive criterion, which is very popular in summing infinite series, is fully legitimate here.

Example 1.4. Sum the series

$$\sum_{i=1}^{\infty} \frac{1}{i^3}$$

with an error less than 10^{-9}. First we compute

$$\sum_{i=1}^{9} \frac{1}{i^3} = 1.19653198567\cdots.$$

Next we apply (1.21) with $f(x) = 1/x^3$ and $m = 10$. Namely, (1.21) should not be used with the low value $m = 1$, but with one that makes R_k small enough (for an acceptable value of k). Our f fulfills the conditions of Theorem 1.3. Verify that the third term in the series of the right-hand side of (1.21) equals

$$-\frac{1}{42}\frac{1}{6!}2520 \times 10^{-8} = -\frac{1}{12} \times 10^{-8} = -0\ 83 \times 10^{-9}$$

Hence, we apply (1.21) with $k = 2$, and we obtain

$$\sum_{i=1}^{\infty} = \frac{1}{i^3} = \sum_{i=1}^{9} + \frac{1}{i^3} + \sum_{i=10}^{\infty} \frac{1}{i^3} = 1.19653198567\cdots$$
$$+ \int_{10}^{\infty} \frac{dx}{x^3} + \frac{1}{2000} + \frac{1}{40000} - \frac{1}{12000000} = 1.20205690234,$$

with an error that is smaller than 0.83×10^{-9}. The actual error is 0.82×10^{-9}.

From this example we see that the error estimate can be very sharp. Another point is that Euler's summation formula may produce a quite accurate result, with almost no effort. To obtain the same accuracy, straightforward numerical summation of the series $\sum i^{-3}$ requires about 22360 terms.

Not all series can be evaluated by Euler's formula in this favorable way. Although the class of series for which the formula is applicable is quite interesting, Euler's method has its limitations. Alternating series should be tackled through Boole's summation method, which is based on the Euler polynomials (see §1.2.2).

Several other summation formulas have been invented to improve the convergence of *slowly convergent series.* Each method has a favorite class of series for which the method is extremely successful. Monotonicity and regularity of the derivatives of the function f that generates the terms of the series always is a good starting point.

To obtain information on how many terms one needs using (1.22) one may use estimates of the Bernoulli numbers. Since the radius of convergence of the series in (1.1) equals 2π, one can use the rough estimate

$$\frac{B_{2k+2}}{(2k+2)!} = \mathcal{O}\left[(2\pi)^{-(2k+2)}\right], \quad \text{as} \quad k \to \infty.$$

This estimate can be refined by using the first series in (1.13). Since the series assumes values between 1 and 2, we have (see also Exercise 1.2)

$$\frac{2}{(2\pi)^{2n}} < (-1)^{n+1}\frac{B_{2n}}{(2n)!} < 2\frac{2}{(2\pi)^{2n}} \quad n = 1, 2, 3, \ldots . \tag{1.23}$$

When also estimates of the derivatives of f are known, much information on R_k of (1.22) may become available.

1.2. Euler Numbers and Polynomials

The *Euler numbers* have a less dominant place in mathematics than those of Bernoulli, although the definitions are quite similar. Again definitions