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Schriftenreihe der Wilhelm Büchner Hochschule

Band 10 / 2023

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Herausgeber Forschungsausschuss der Wilhelm Büchner Hochschule
15.03.2023

Wilhelm Büchner Hochschule

Impressum

ISSN (Online) 2751-0514

Die Deutsche Nationalbibliothek verzeichnet diese Publikation in der Deutschen Nationalbibliografie; detaillierte bibliografische Daten sind im Internet über http://dnb.d-nb.de abrufbar.

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Herausgeber: Forschungsausschuss der Wilhelm Büchner Hochschule
Redaktion: Dr. Marcel Heber
Layout und Satz: Philipp Thißen
Einbandentwurf : Gerhard Kienzle
Projektkoordination: Prof. Dr. Klaus Fischer

Gedruckt auf säurefreiem und chlorfrei gebleichtem Papier.

Introduction to Extrapolation Algorithms in Numerical Analysis including New Results

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Zusammenfassug Die Intention der vorliegenden Publikation ist zweifach: Im ersten Teil geben wir einen Überblick über Extrapolationsverfahren in der Numerischen Mathematik, die einen modernen Ansatz zur Konvergenzbeschleunigung darstellen. Voraussetzung für die Anwendbarkeit solcher Verfahren ist, dass die Folge, deren Konvergenz beschleunigt werden soll, eine sogenannte asymptotische Entwicklung besitzt. Daher wird auch dieses Thema im Folgenden behandelt. Der zweite Teil der Publikation ist dem Problem der numerischen Berechnung der Matrix-Exponentialfunktion durch Extrapolation gewidmet. Wir greifen einen vor einigen Jahren in [Walz2] erstmals vorgestellten Algorithmus auf und präsentieren die Ergebnisse ausführlicher numerischer Tests.

Keywords: Extrapolationsverfahren, asymptotische Entwicklung, Matrix-Exponentialfunktion

Abstract The aim of the present publication is twofold: In the first part we give a survey on extrapolation methods in Numerical Analysis, which establish a modern technique for convergence acceleration. A prerequisite for the application of extrapolation is the existence of a so-called asymptotic expansion for the sequence under consideration. Therefore, also this topic is treated on the following pages. The second part of the paper is devoted to the problem of computing the matrix exponential function by means of extrapolation. We resume an algorithm presented some years ago in [Walz2] and present the results of extensive numerical tests.

Keywords: extrapolation methods, asymptotic expansion, matrix exponential function

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Foreword

The question whether a given sequence converges or not is a fundamental topic in mathematical analysis throughout the centuries, beginning in some sense with Archimedes of Syracuse ([Arch]), and highlighted later on by giants such as Newton, Leibniz and Cauchy, to quote only a very few of them.
In classical analysis it is irrelevant, how fast the sequence under consideration converges, the main thing is it converges anyway. For example, it is well known that the series

$$\sum_{i=1}^{\infty} \frac{1}{i^{1+\varepsilon}}$$

converges for each $\varepsilon > 0$. But if you choose ε very close to zero, you will have to calculate a very, very large number of summands to get near to the limit value. But as I said: In classical analysis this does not matter at all, and classical analysists are satisfied with the sheer convergence anyway.
In contrast to this, in Numerical Analysis the speed of convergence is of fundamental interest, since the goal is to compute the limit value of the sequence fast.
Let us look at two examples:
The so-called *Babylonian Method* for calculating $\sqrt{2}$ consists in computing the sequence

$$x_{i+1} = \frac{1}{2}\left(x_i + \frac{2}{x_i}\right), i = 0, 1, 2, \ldots,$$

starting e.g. with $x_0 = 1.5$. It is well known that this sequence converges very fast, e.g. already the third iteration

$$x_3 = 1.41421356237.....$$

is correct in all decimals shown here.
A familiar method for computing *Euler's constant* e is to calculate the numbers

$$s_n = \left(1 + \frac{1}{n}\right)^n$$

for increasing values of n, since

$$\lim_{n\to\infty} \left(1 + \frac{1}{n}\right)^n = \mathrm{e}.$$

But here, the convergence is quite slow, e.g.

$$s_{100} = 2.70481......$$

is correct only in one decimal!

So what to do? Now, in these situations there is need for *convergence acceleration algorithms*, and this is the reason why they establish a fundamental research field in Numerical Analysis.
A type of convergence acceleration algorithms which has gained interest in the last decades are so-called *extrapolation methods*, which are the topic of this paper. There is already a vast literature on this (see e.g. [Brez1], [Brez2], [BrRe], [Walz9], [Walz10] and the references therein), but the specific problem of com-

puting the matrix exponential by extrapolation is to the best of my knowledge not treated very well, as far as numerical results are concerned.

So the aim of this paper is twofold. In the first part I give a very brief overview over extrapolation methods, in particular, I want to give an impression, in which different fields of mathematics they can be applied. The second part is devoted to the problem of computing the so-called matrix exponential (function) by extrapolation methods.

Here also new results, in particular outcomes of extensive numerical calculations, are given. These were obtained in the context of the research project „Matrix Exponential“ of Wilhelm Büchner Hochschule. I am very thankful to the Research Committee for having had the opportunity to work on this project for some months, and I also want to thank Florian Bierbaum, who established the software to do the numerical calculations.

So, have at least that amount of fun with reading the following pages as I had with writing them!

Summer 2022, Guido Walz

1 Introduction and First Examples

In this chapter we give an introduction to convergence acceleration by extrapolation methods. A prerequisite for the application of these methods is that the sequence under consideration (i.e., the sequence whose convergence should be accelerated) possesses a so-called asymptotic expansion, a term which is also treated on the following pages.
Moreover, we present some examples from different parts of Numerical Analysis.

1.1 Fundamental Definitions

We start directly with the definition of the term asymptotic expansion.

Definition 1.1
Let there be given a (finite or infinite) sequence of real numbers $R = \{r_m\}$ with the property

$$0 < r_1 < r_2 < \cdots ,$$

i.e., R is positive and strictly increasing.
A sequence $\{s_n\}$ is said to possess an asymptotic expansion of order M with limit c_0 and with respect to R, if for each n large enough, s_n can be written in the form

$$s_n = c_0 + \sum_{m=1}^{M} \frac{c_m}{n^{r_m}} + o(n^{-r_M}) \tag{1.1}$$

with coefficients c_m, which are independent of n; here, o denotes the well-known Landau symbol.
If (1.1) holds for each $M \in \mathbb{N}$, we write

$$s_n = c_0 + \sum_{m=1} \frac{c_m}{n^{r_m}} \tag{1.2}$$

for short.

Remark
In a more general context, asymptotic expansions of the type (1.1) are denoted as special logarithmic asymptotic expansions, in contrast to the so-called geometric expansions, see [Walz9]. In this paper we will concentrate on the first type of expansions.

It is not easy to give a first quick example for that, since the proof of the existence of an asymptotic expansion is not easy in most cases. However, the following is not too difficult to see (cf. also [Walz6]):

Example 1.1
Consider some real function f, which has derivtives of arbitrary order in some definition range D, and fix some $x \in D$, such that $[x, x+1]$ also belongs to D. Then the sequence $s_n = s_n(x)$, defined by

$$s_n(x) = n \cdot (f(x + \frac{1}{n}) - f(x)) \tag{1.3}$$

possesses an asymptotic expansion with limit $f'(x)$ and with respect to the set $\mathbb{N}$ of arbitrary order, i.e.

$$s_n(x) = f'(x) + \sum_{m=1} \frac{c_m(x)}{n^m}, \tag{1.4}$$

where the coefficients c_m may depend on x, but not on n.

Proof: To prove this assertion we make use of the Taylor series of f and apply it to $f(x + \frac{1}{n})$. This yields

$$f(x + \frac{1}{n}) = \sum_{j=0}^{\infty} \frac{f^{(j)}(x)}{j! n^j}.$$

Therefore,

$$f(x + \frac{1}{n}) - f(x) = \sum_{j=1}^{\infty} \frac{f^{(j)}(x)}{j! n^j}$$

and multiplication with n proves (1.4). □
With the same approach one can show (cf. [Rutish]):
Under the assumptions from above, the sequence $\widetilde{s}_n(x)$, defined by

$$\widetilde{s}_n(x) = \frac{n}{2} \cdot (f(x + \frac{1}{n}) - f(x - \frac{1}{n})) \tag{1.5}$$

possesses an asymptotic expansion with limit $f'(x)$ and with respect to the set $2\mathbb{N}$ of arbitrary order, i.e.

$$\widetilde{s}_n(x) = f'(x) + \sum_{m=1} \frac{c_m(x)}{n^{2m}}. \tag{1.6}$$

■

Further examples and numerical illustrations will be given soon.
We now proceed to the central topic of this paper, namely the acceleration of convergence of a given sequence, which is known to possess an asymptotic expansion of the above type:

Theorem 1.1
Let $\{s_n\}$ be a sequence which possesses an asymptotic expansion of order M with respect to a given sequence $R = \{r_m\}$, and apply the following linear extrapolation process:

- *Choose a maximal index $k_{max} < M$*
- *Compute*
$$y_i^{(0)} = s_{2^i}$$
for $i = 0, 1, \ldots, k_{max}$.
- *Compute*
$$y_i^{(k)} = y_{i+1}^{(k-1)} + \frac{1}{2^{r_k} - 1} \cdot (y_{i+1}^{(k-1)} - y_i^{(k-1)}) \tag{1.7}$$
for $k = 1, 2, \ldots, k_{max}$ and $i = 0, 1, \ldots, k_{max} - k$.

Then for each $k \leq k_{max}$, the sequences $\{y_i^{(k)}\}$ possess an asymptotic expansion of the form
$$y_i^{(k)} = c_0 + \sum_{m=k+1}^{M} \frac{c_m^{(k)}}{n^{r_m}} + o(n^{-r_M}) \tag{1.8}$$

So, the extrapolated sequences converge to the same limit as the initial one, but do this faster, namely with order $O(n^{-r_{k+1}})$ instead of $O(n^{-r_1})$.

Remark
Alternatively, the computation in (1.7) can be done in the form

$$y_i^{(k)} = \frac{2^{r_k} y_{i+1}^{(k-1)} - y_i^{(k-1)}}{2^{r_k} - 1}$$

In practice, the results of the extrapolation process usually are displayed in a triangular scheme, also denoted as Romberg scheme oder Romberg table, see Table 1.1.

$$\begin{array}{ccccc}
y_0^{(0)} & & & & \\
 & y_0^{(1)} & & & \\
y_1^{(0)} & & \ddots & & \\
 & \vdots & & y_0^{(k_{max}-1)} & \\
\vdots & & \vdots & & y_0^{(k_{max})} \\
 & \vdots & & y_1^{(k_{max}-1)} & \vdots \\
\vdots & & \cdot^{\cdot^{\cdot}} & \vdots & \\
 & y_{k_{max}-1}^{(1)} & \vdots & & \\
y_{k_{max}}^{(0)} & \vdots & & & \\
\vdots & & & &
\end{array}$$

Table 1.1: Romberg table

The value $y_0^{(k_{max})}$ is taken as an approximation to the desired value c_0.

Example 1.2
a) As a first example we apply the extrapolation process to the sequence (1.3) given above, which possesses an asymptotic expansion with respect to $R = \mathbb{N}$ and limit $f'(x)$. Just for illustration, we choose $f(x) = \ln(x)$ and $x = 2$ with the true value $f'(2) = 0.5$. Table 1.2 is built as shown in Table 1.1, with $k_{max} = 4$. I.e., in the first column you see the values of

$$s_n(2) = n \cdot (\ln(2 + \frac{1}{n}) - \ln(2)) \ \text{ for } n = 1, 2, 4, 8, 16,$$

and in the next columns the results of the extrapolation process, which reads here

$$y_i^{(k)} = y_{i+1}^{(k-1)} + \frac{1}{2^k - 1} \cdot (y_{i+1}^{(k-1)} - y_i^{(k-1)}) \tag{1.9}$$

with $y_i^{(0)} = s_{2^i}(2)$. The effect of the extrapolation is evident.

0,40546511				
	0,48710910			
0,44628710		0,49893321		
	0,49597718		0,49995051	
0,47113214		0,49982335		0,49999877
	0,49886181		0,49999575	
0,48499697		0,49997420		
	0,49969610			
0,49234654				

Table 1.2: Example 1.2 a)

b) Maybe even more impressive is the extrapolation based on the sequence $\widetilde{s}_n$ defined in (1.5). Here, with $k_{max} = 4$ the full 8-digit-accuracy is obtained. Since here $r_m = 2m$ for all m, the extrapolation process reads

$$y_i^{(k)} = y_{i+1}^{(k-1)} + \frac{1}{4^k - 1} \cdot (y_{i+1}^{(k-1)} - y_i^{(k-1)}).$$

The results are shown in Table 1.2.

$0,54930614$				
	$0,49799878$			
$0,51082562$		$0,50002312$		
	$0,49989660$		$0,49999993$	
$0,50262886$		$0,50000029$		$0,50000000$
	$0,49999381$		$0,50000000$	
$0,50065257$		$0,50000000$		
	$0,49999962$			
$0,50016286$				

Table 1.3: Example 1.2 b)

■

More examples will follow throughout the paper.

1.2 Overview and Historical Remarks

It should be emphasized here once more, that extrapolation is a very efficient method for convergence acceleration, and the only prerequisite for its application is the fact that the sequence under consideration must possess an asymptotic expansion. It is by no means of interest, in which context and by which numerical process this sequence was computed. This implies that extrapolation nowadays is applied in various fields of Numerical Analysis. In this section we give a very brief overview on these fields. For the sake of brevity we will, with a few exceptions, only indicate the topics without giving specific formulas or examples and refer the interested reader to textbooks and survey articles such as [Brez2], [BrRe], [Dela], [Joyce], [Walz9], [Walz10] and further references therein.

1.2.1 Integration of functions

The modern interest in extrapolation methods started in 1955 with Romberg's paper entitled „Vereinfachte numerische Integration“ (Simplified numerical intgration) ([Romb]). Romberg's method, which is in fact an extrapolation method, is based on the fact, that the well-known trapezoidal rule possesses an asymptotic expansion. The exact assertion is as follows:

Theorem 1.2
For some interval $[a,b]$ and $r \in \mathbb{N}_0$, let $f \in C^{2r+1}[a,b]$. Suppose we want to approximate the value

$$I_a^b(f) = \int_a^b f(x)\,dx$$

by means of the trapezoidal rule with n subintervals, $n \in \mathbb{N}$, i.e. by the formula

$$T_n(f) = \frac{b-a}{n}\left(\frac{1}{2}f_0 + \sum_{\nu=1}^{n-1} f_\nu + \frac{1}{2}f_n\right),$$

where

$$x_\nu = a + \nu \cdot \frac{b-a}{n} \quad \textit{and} \quad f_\nu = f(x_\nu) \quad for \;\; \nu = 0,\ldots,n\;.$$

Then the sequence $\{T_n(f)\}$ possesses an asymptotic expansion with limit $I_a^b(f)$ of order r with respect to the set $R = \{2,4,6,\dots\}$; more precisely, we have

$$T_n(f) \;=\; I_a^b(f) \;+\; \sum_{m=1}^{r} \frac{c_m}{n^{2m}} \;+\; o(n^{-2r})\,. \tag{1.10}$$

The assertion makes use of Euler's summation formula ([Euler]), the full proof can be found in many textbooks on Numerical Ananlysis, or. e.g. in [Walz9].
The existence of an asymptotic expansion justifies the application of an extrapolation process, which reads in this case as follows:

Theorem 1.3 ([Romb])
Consider the numerical integration of some function $f \in C^{2r+1}[a,b]$, $r \in \mathbb{N}_0$. To do this, define, for natural numbers $n_i = 2^i$, the trapezoidal values

$$T_i^0 := T_{n_i}(f) = \frac{b-a}{n_i}\left(\frac{1}{2}f(a) + \sum_{\nu=1}^{n_i-1} f\Big(a+\nu\,\frac{b-a}{n_i}\Big) + \frac{1}{2}f(b)\right) \tag{1.11}$$

and the midpoint values

$$U_i^0 := U_{n_i}(f) = \frac{b-a}{n_i}\cdot\sum_{\nu=0}^{n_i-1} f\Big(a+(2\nu+1)\,\frac{b-a}{2n_i}\Big), \tag{1.12}$$

both of which's error is of order n_i^{-2}.
Then the following holds:
1. For each n,

$$T_{2n}(f) \;=\; \frac{T_n(f)+U_n(f)}{2}$$

holds, which obviously reduces the amount of work for the computation of the sequences $\{T_n(f)\}$ and $\{U_n(f)\}$ considerably.
2. If we define new sequences $\{T_i^k\}$ and $\{U_i^k\}$ through the iterative processes

$$T_i^k \;:=\; T_{i+1}^{k-1} + \frac{T_{i+1}^{k-1} - T_i^{k-1}}{4^k-1}\,, \quad \textit{for } k = 1,2,\dots, \textit{ and } i = 0,1,\dots \tag{1.13}$$

and analogously

$$U_i^k \;:=\; U_{i+1}^{k-1} + \frac{U_{i+1}^{k-1} - U_i^{k-1}}{4^k-1}\,, \quad \textit{for } k = 1,2,\dots, \textit{ and } i = 0,1,\dots, \tag{1.14}$$

then the error of $\{T_i^k\}$ as well as that of $\{U_i^k\}$ is of order $4^{-(k+1)i}$, and thus, for each k, the sequences of stage k converge faster than those of stage $(k-1)$.
This is Romberg's method for numerical quadrature: To compute the integral $\int_a^b f$ numerically, take the (rather crude) approximations T_i^0 and/or U_i^0 for $i = 0,1,2,\dots$, and then apply the convergence accelerating processes (1.13) resp. (1.14).
Due to the historical importance we present one short numerical example: Computing of the integral

$$\int_1^2 \frac{1}{x}dx \tag{1.15}$$

using the trapezoidal rule combined with the extrapolation process (1.13).
The results are shown in Table 1.4 and should be compared with the true value $\ln(2) = 0,69314718....$

$0,75000000$				
	$0,69444444$			
$0,70833333$		$0,69317461$		
	$0,69325397$		$0,69314748$	
$0,69702381$		$0,69314790$		$0,69314718$
	$0,69315453$		$0,69314718$	
$0,69412185$		$0,69314719$		
	$0,69314765$			
$0,69339120$				

Table 1.4: Calculation of $\int_1^2 \frac{1}{x}\,dx$ using (1.13); the first column shows the results of the trapezoidal rule

1.2.2 Numerical computation of π and e

It is remarkable that common methods for the numerical computation of the two most prominent constants in mathematics, namely π and e, turn out to produce sequences which possess an asymptotic expansion.
We start with some remarks on the numerical computation of π: The following construction dates back to the age of Archimedes, see [Arch]; it is well-described in many publications on numerical quadrature and related topics.

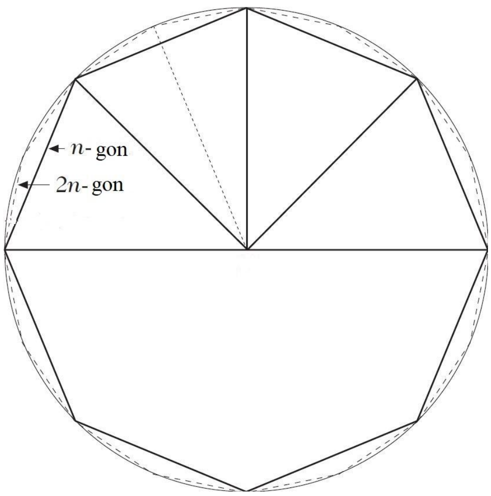

Fig. 1.1: Unit circle with inscribed regular polygons

Let A_n denote the area of a regular polygon with n vertices, n-gon for short, which is inscribed into the unit circle. By intuition it is clear that

$$\lim_{n\to\infty} A_n \;=\; \pi \;, \tag{1.16}$$

and this fact was used by Archimedes for his method of approximating π. He computed one by one the numbers $A_6, A_{12}, A_{24}, A_{48}$, and so on, until the desired accuracy was reached, and took the last value as an approximation for π. (In fact, he did even more, namely he also computed the areas of the corresponding circumscribed polygons, say U_n, and therefore obtained in each step an inclusion of the true value, i.e. $A_n < \pi < U_n$ for all n.)
It is remarkable that he did not increase the number n somehow, but he precisely doubled it in each step, which is an interesting connection to the modern approach by extrapolation methods.
Let us now analyze relation (1.16) in more detail. First, a little computation shows that, for $n \in \mathbb{N}$,

$$A_{2n} \;=\; n \cdot \sin\left(\frac{\pi}{n}\right), \tag{1.17}$$

and, using the series expansion of the sine function, we obtain

$$A_{2n} \;=\; \pi \;+\; \sum_{m=1} \frac{c_m}{n^{2m}}$$

with

$$c_m \;=\; (-1)^m \cdot \frac{\pi^{2m+1}}{(2m+1)!} \quad \text{for all } \; m \in \mathbb{N}\,,$$

and recognize that $\{A_n\}$ possesses an asymptotic expansion of arbitrary order with limit π and $r_m = 2m$ for all m.
Of course it would make no sense to approximate π by the sequence $\{A_n\}$, if these numbers would have to be computed via (1.17), thus using the number π itself. But fortunately it is possible to calculate certain subsequences of $\{A_n\}$ recursively, which is stated in the following result:
Define the sequence $\{Y_i\}$ through the recursion formula

$$Y_{i+1} \;:=\; Y_i \cdot \frac{\sqrt{2}}{\sqrt{1+\sqrt{1-(Y_i/2^i)^2}}} \qquad \text{for } i = 0, 1, 2, \ldots, \tag{1.18}$$

with $Y_0 = 2$. Then for all $i \in \mathbb{N}$ the identity

$$Y_i \;=\; A_{2^{i+2}}$$

holds; in other words, equation (1.17) yields a recursion formula for the computation of the sequence $\{A_{2^i}\}$.
For many centuries the computation of numbers A_n was the most widespread method for the computation of π, and the only progress that was made consisted in increasing the number of vertices of the respective polygons. For example, Ludolf van Ceulen (= from Cologne) in the year 1610 obtained 35 digits of π by calculating the area A_n of the regular polygon with $n = 2^{62}$ vertices!
The first methodical advance is due to Ch. Huygens ([Huy]) in 1654; using geometrical arguments, he showed that the sequence $\{T_n\}$, defined by

$$T_n = \frac{4A_{2n} - A_n}{3}$$

converges faster to the limit π than the sequence $\{A_n\}$ itself does. So, Huygens found out the first step (but only the first) of the extrapolation procedure (1.7) as a convergence accelerating method in this special case.

The next milestone in the history of extrapolation methods is, without any doubt, the booklet of Saigey [Saigey] from 1859, which unfortunately was overlooked for more than a century and was rediscovered in 1984 by Dutka [Dutka]. Saigey developed, with purely analytical methods, in particular without refering to Archimedes or Huygens, the existence of an asymptotic expansion for the sequence $\{A_n\}$ from above, i.e. he proved (with a slight change of notations)

$$A_n \;=\; \pi + \frac{c_1}{n^2} + \frac{c_2}{n^4} + \frac{c_3}{n^6} + \cdots \;,$$

where the c_ν are fixed coefficients, and then derived from this relation his „higher approximations“ to π, which turn out to be nothing else than the results of the lex process: Considering $\{A_n\}$ as the sequence of *first approximations*, he defines the *second approximations*,

$$\tilde{A}_n \;:=\; A_{2n} + \frac{1}{3} \cdot (A_{2n} - A_n) \;,$$

the *third approximations*,

$$B_n \;:=\; \tilde{A}_{2n} + \frac{1}{15} \cdot (\tilde{A}_{2n} - \tilde{A}_n) \;,$$

the *fourth approximations*,

$$C_n \;:=\; B_{2n} + \frac{1}{63} \cdot (B_{2n} - B_n) \;,$$

and so on. So, Saigey was the very first who developed a special case of the extrapolation process (1.13) in iterative form; note that this was almost precisely 100 years before Rombergs paper appeared.

Another very prominent number in mathematics is Euler's constant e. There exist dozens of numerical methods for the computation of this number or, more general, for the copmputation of the exponential function $\exp(x) = \mathrm{e}^x$, $x \in \mathbb{C}$. One of them is as follows:

Theorem 1.4
Let, for arbitrary $n \in \mathbb{N}$ and $x \in \mathbb{C}$,

$$s_n(x) = \left(1 + \frac{x}{n}\right)^n . \tag{1.19}$$

Then

$$\lim_{n\to\infty} s_n(x) \;=\; \exp(x). \tag{1.20}$$

In particular,

$$\lim_{n\to\infty} \left(1 + \frac{1}{n}\right)^n = e. \tag{1.21}$$

Even more, it can be shown that the sequence $s_n(x)$ defined in (1.19) possesses the asymptotic expansion

$$s_n(x) = \exp(x) + \sum_{m=1} \frac{c_m(x)}{n^m} \tag{1.22}$$

of arbitrary order, which sharpens (1.20) considerably.
Therefore, the extrapolation process can be applied. A first example is given here (see Table 1.5), setting $k_{max} = 4$ and $x = \frac{1}{2}$, thus approximating the value

$$\exp\left(\frac{1}{2}\right) = 1.648721....$$

$1,500000$				
	$1,625000$			
$1,562500$		$1,646484$		
	$1,641113$		$1,648605$	
$1,601806$		$1,648340$		$1,648718$
	$1,646533$		$1,648711$	
$1,624170$		$1,648664$		
	$1,648131$			
$1,636151$				

Table 1.5: Approximation of $\exp(\frac{1}{2})$ using extrapolation

In Chapter 2 this will be applied to square matrices which will provide new results on the matrix exponential.

1.2.3 Numerical differentiation

In the previous section we had already encountered an example (Example 1.1) for the approach we are going to present now: It was shown that the application of two specific first-order divided differences, the forward difference and the central difference, to a function g produces asymptotic expansions with limit function g'. In the following we shall generalize this result considerably. Most of the following results were first presented in [Walz6] and [Walz8].
We first have to learn some elementary facts on divided differences:

Definition 1.2
For some $\nu \in \mathbb{Z}$ and $m \in \mathbb{N}_0$, let there be given a set of pairwise distinct numbers $\{x_\nu, \ldots, x_{\nu+m}\}$ and a function g, which is defined at these points.
Then the $m-$th order divided difference $\Delta(x_\nu, \ldots, x_{\nu+m}; g)$ of g with respect to the points $x_\nu, \ldots, x_{\nu+m}$ is defined recursively by

$$\begin{aligned}
\Delta(x_j; g) &= g(x_j) \qquad \text{for } j = \nu, \ldots, \nu+m, \\
\Delta(x_j, \ldots, x_{j+k}; g) &= \frac{\Delta(x_j, \ldots, x_{j+k-1}; g) - \Delta(x_{j+1}, \ldots, x_{j+k}; g)}{x_j - x_{j+k}} \\
&\quad \text{for } k = 1, \ldots, m \text{ and } j = \nu, \ldots, \nu+m-k.
\end{aligned}$$

In almost every textbook on numerical analysis, one can find the proofs of the following elementary properties of the operator Δ:

Theorem 1.5
a) The divided difference $\Delta(x_\nu,\ldots,x_{\nu+m};g)$ *can be written in the form*

$$\Delta(x_\nu,\ldots,x_{\nu+m};g) \;=\; \sum_{\mu=\nu}^{\nu+m} \frac{g(x_\mu)}{\omega^m_{\nu,\mu}}$$

with

$$\omega^m_{\nu,\mu} \;=\; \prod_{\substack{\lambda=\nu\\ \lambda\neq\mu}}^{\nu+m} (x_\mu - x_\lambda)\,.$$

b) Application of the divided difference operator Δ *to the monomial* $p_j(x) := x^j$ *yields*

$$\Delta(x_\nu,\ldots,x_{\nu+m};p_j) \;=\; \begin{cases} 0\,, & \text{for } j=0,\ldots,m-1\\ 1\,, & \text{for } j=m, \end{cases}$$

i.e. Δ *annihilates the polynomial space* Π_{m-1}. *In fact,* Δ *is even uniquely determined by this property, see [BrWa].*
Now let $[x_\nu,\ldots,x_{\nu+m}]$ denote the smallest interval containing the points $x_\nu,\ldots,x_{\nu+m}$, and consider some $g\in C^m[x_\nu,\ldots,x_{\nu+m}]$. Then it is known that, if all points $x_\nu,\ldots,x_{\nu+m}$ collapse to one, say ξ, $\Delta(x_\nu,\ldots,x_{\nu+m};g)$ converges to $\frac{g^{(m)}(\xi)}{m!}$.
In the case of equidistant points, the following fundamental lemma sharpens this result considerably:

Theorem 1.6 ([Walz8])
Fix some arbitrary index $k\in\{\nu,\ldots,\nu+m\}$*, and consider, for* $n\in\mathbb{N}$*, the sequence of equidistant points* $\{x^{(n)}_\nu,\ldots,x^{(n)}_{\nu+m}\}$*, defined through*

$$x^{(n)}_{k+j} := x_k + \frac{j}{n}\,,\quad j=\nu-k,\ldots,\nu-k+m\,.$$

Furthermore, assume that the function g *belongs to the differentiability class* $C^{r+1}[x^{(1)}_\nu,\ldots,x^{(1)}_{\nu+m}]$ *for some* $r>m$.
Then the sequence $\{\Delta(x^{(n)}_\nu,\ldots,x^{(n)}_{\nu+m};g)\}_{n\in\mathbb{N}}$ *possesses the following asymptotic expansion of order* $r-m$*:*

$$\Delta(x^{(n)}_\nu,\ldots,x^{(n)}_{\nu+m};g) = \frac{g^{(m)}(x_k)}{m!} + \sum_{j=1}^{r-m} \frac{c_j}{n^j} + o(n^{m-r}).$$

The result of Theorem 1.6 has a variety of applications in numerical analysis, the most obvious of which being the numerical differentiation of functions. This will be treated as an example in the rest of this subsection.
We still have the possibility to choose the index k appropriately, and the most promising (and popular) choices are $k=\nu$ and, for even values of m, $k=\nu+\frac{m}{2}$, which lead to the so-called forward resp. central difference operators:

Definition 1.3
Fix some value $x\in\mathbb{R}$. Then, adopting the notations from above, we call the operator

$$\delta^f_n(g;m,x) \;:=\; \Delta(x,x+\frac{1}{n},\ldots,x+\frac{m}{n};g) \tag{1.23}$$

the m^{th} forward difference of g, and

$$\delta_n^c(g;m,x) \;:=\; \Delta(x-\frac{m}{2n},x-\frac{m-2}{2n},\ldots,x+\frac{m-2}{2n},x+\frac{m}{2n};g) \tag{1.24}$$

the m^{th} central difference of g. Note that we have on the right hand sides of (1.23) and (1.24) both times divided differences of order m.

We can now apply Theorem 1.6 to the operators $\delta_n^f(g;m,x)$ and $\delta_n^c(g;m,x)$, thus obtaining the main result of this subsection concerning the numerical differentiation of a function; in a different approach, i.e. without using divided differences, and with a completely different proof, the second part of the following result (concerning $\delta_n^c(g;m,x)$) goes back to Rutishauser [Rutish] (for $m=1$) and Ström [Ström].

Theorem 1.7 ([Walz8])
Adopt the notations and assumptions from Theorem 1.6. Then the following results hold:
a) The forward difference operator $\delta_n^f(g;m,x)$ possesses an asymptotic expansion of the form

$$\delta_n^f(g;m,x) \;=\; \frac{g^{(m)}(x)}{m!}+\sum_{j=1}^{r-m}\frac{c_j(x)}{n^j}+o(n^{m-r}).$$

b) The central difference operator $\delta_n^c(g;m,x)$ possesses an asymptotic expansion of the form

$$\delta_n^c(g;m,x) \;=\; \frac{g^{(m)}(x)}{m!}+\sum_{j=1}^{r-m}\frac{\gamma_j(x)}{n^j}+o(n^{m-r}) \tag{1.25}$$

with

$$\gamma_j \;=\; 0 \quad \text{for } j \text{ odd},$$

i.e. the expansion in (1.25) contains only even powers of n.

Example 1.3
We conclude this subsection with a numerical example. Let $g(x)=\sin(x)$, $m=2$ and $x=\frac{\pi}{3}$. So, we consider the second derivative of the sine function in $x=\frac{\pi}{3}$, which is exactly

$$-\sin(\frac{\pi}{3})=-\frac{\sqrt{3}}{2}=-0.86602540..... \tag{1.26}$$

We will make use of the central difference operator δ_n^c, which takes here the form

$$\begin{aligned}\delta_n^c(\sin,2,\frac{\pi}{3}) &= \Delta\left(\frac{\pi}{3}-\frac{1}{n},\frac{\pi}{3},\frac{\pi}{3}+\frac{1}{n}\right)\\ &= \frac{n^2}{2}\left(\sin\left(\frac{\pi}{3}-\frac{1}{n}\right)-2\sin\left(\frac{\pi}{3}\right)+\sin\left(\frac{\pi}{3}+\frac{1}{n}\right)\right)\end{aligned}$$

We computed these expressions for some values of n and obtained

$$\begin{aligned}
\delta_2^c(\sin, 2, \frac{\pi}{3}) &= -0,424066445 \\
\delta_4^c(\sin, 2, \frac{\pi}{3}) &= -0,430762121 \\
\delta_8^c(\sin, 2, \frac{\pi}{3}) &= -0,432449177 \\
\delta_{16}^c(\sin, 2, \frac{\pi}{3}) &= -0,432871766 \\
\delta_{32}^c(\sin, 2, \frac{\pi}{3}) &= -0,432977464
\end{aligned}$$

Note that, according to (1.25), these numbers are approximations to the halfed second derivative, which reads -0.43301270.
Applying now extrapolation to these values yields the following table, which looks quite satisfactory.

$-0,424066445$		
	$-0,43299401$	
$-0,430762121$		$-0,43301270$
	$-0,43301153$	
$-0,432449177$		$-0,43301270$
	$-0,43301263$	
$-0,432871766$		$-0,43301270$
	$-0,43301270$	
$-0,432977464$		

Table 1.6: Approximation of $\sin''(\frac{\pi}{3}) = -0.43301270$ using the central difference operator combined with extrapolation

■

1.2.4 Approximation of functions

In this section we summarize some results on the approximation of special functions using sequences which turn out to possess an asymptotic expansion. We use two different approaches; the results shown in this section were developed in [Walz1], see also [Walz9]. There one can also find the proofs of the following theorems.

1.2.4.1 Partial Products of Infinite Products

Let us begin with the following special case of the famous Weierstraß factorization theorem:

Theorem 1.8
Consider some arbitrary entire function f with $f(0) \neq 0$, and denote the set of its zeros by $\{a_\nu\}$. Furthermore, let there exist some natural number r, such that the infinite series

$$\sum_{\nu=1}^{\infty} \left(\frac{1}{|a_\nu|}\right)^{r+1}$$

converges and set, for all ν in $\mathbb{N}$:

$$E_\nu(z) \;:=\; \left(1 - \frac{z}{a_\nu}\right) \cdot \exp\left(\sum_{j=1}^{r} \frac{1}{j} \left(\frac{z}{a_\nu}\right)^j\right) .$$

Then there exists an entire function g, such that for all $z \in \mathbb{C}$ the equality

$$f(z) \;=\; \exp(g(z)) \cdot \prod_{\nu=1}^{\infty} E_\nu(z)$$

holds.
The connection of this theorem with our considerations on asymptotic expansions is given by the following Theorem 1.9, which says that - under certain assumptions on the set $\{a_\nu\}$ - the sequence of partial products

$$\sigma_n(z) \;:=\; \exp(g(z)) \cdot \prod_{\nu=1}^{n} E_\nu(z) \tag{1.27}$$

possesses an asymptotic expansion with limit $f(z)$.

Theorem 1.9 ([Walz1], [Walz9])
Adopt the notations and assumptions of Theorem 1.8, and assume in addition that for all $j \geq r+1$ the partial sums of the series $\sum_{\nu=1}^{\infty} \left(\frac{1}{a_\nu}\right)^j$ possess an asymptotic expansion i.e., there exist numbers $\eta(j)$ and $c_\mu(j)$, such that

$$\sum_{\nu=1}^{n} \left(\frac{1}{a_\nu}\right)^j \;=\; \eta(j) \;+\; \sum_{\mu=1} \frac{c_\mu(j)}{n^{\rho_\mu(j)}}. \tag{1.28}$$

Then also the partial products in (1.27) possess an asymptotic expansion of the form

$$\sigma_n(z) \;=\; f(z) \;+\; \sum_{\mu=1} \frac{\gamma_\mu(z)}{n^{\lambda_\mu}} ,$$

where the λ_μ are sums of certain $\rho_\mu(j)'s$, and in particular $\lambda_1 = \rho_1(r+1)$.

Example 1.4
With $\Gamma(z)$ denoting the usual Gamma-function, we consider the entire function

$$f(z) \;:=\; \frac{1}{z \cdot \Gamma(z)} .$$

It is well-known that the zeros of f are precisely the negative integers, each of them having multiplicity one. Therefore, the assumptions in Weierstraß' factorization theorem are satisfied, and since

$$\sum_{\nu=1}^{\infty} \frac{1}{\nu^2} < \infty,$$

we may take $r = 1$. Furthermore, the exponential function in front of the Weierstraß product can be chosen to be $\exp(g(z)) := \exp(Cz)$ with the Euler-Mascheroni constant C.
In order to check the applicability of Theorem 1.9, we have to look onto the asymptotic behaviour of the sums $\sum_{\nu=1}^{n} \frac{1}{(-\nu)^j}$ for all $j \in \mathbb{N}$, $j \geq 2$. It can be shown (see e.g. [Walz9]) that

$$\sum_{\nu=1}^{n} \frac{1}{(-\nu)^j} = (-1)^j \zeta(j) + \sum_{\mu=1} \frac{c_\mu(j)}{n^{j-2+\mu}},$$

i.e. a relation of the type (1.28) holds. Therefore we may apply Theorem 1.9 to the function f under consideration and obtain the following result: The partial products

$$\sigma_n(z) := \exp(Cz) \cdot \prod_{\nu=1}^{n} \left(\left(1 + \frac{z}{\nu}\right) \exp\left(\frac{-z}{\nu}\right) \right)$$

of the Weierstraß product for the function f possess the asymptotic expansion

$$\sigma_n(z) = \frac{1}{z\Gamma(z)} + \sum_{\mu=1} \frac{\gamma_\mu(z)}{n^\mu}.$$

■

1.2.4.2 Use of Taylor's Expansion

The method for the numerical computation of π presented in Section 1.2.2 can be modified and generalized in many ways; in the present subsection we use the idea behind it in order to construct asymptotic expansions for real functions, which are invertible on a certain interval and possess there a series expansion. Most of the material presented in this subsection comes from the author's doctoral thesis [Walz1], see also [Walz9], but special cases of it can already be found in the papers of Rutishauser ([Rutish]) and Filippi ([Filippi]).
We begin with the following illustrative example, which is a direct generalization of the method for computing π.

Example 1.5
Our aim is to construct an asymptotic expansion with limit

$$f(x) = \arcsin(x) \qquad \text{for } x \in [-1, 1].$$

In this special case we know explicitly the series expansion for the inverse $f^{-1}(y) = \sin(y)$ of f, namely

$$f^{-1}(y) \;=\; y \;+\; \sum_{\nu=1}^{\infty} \frac{(-1)^{\nu}}{(2\nu+1)!} \cdot y^{2\nu+1} \tag{1.29}$$

for all $y \in \mathbb{R}$. So, if we define, for $n \in \mathbb{N}$ and $x \in [-1,1]$

$$\sigma_n(x) \;:=\; n \cdot \sin\left(\frac{\arcsin(x)}{n}\right), \tag{1.30}$$

we immediately get from (1.29) the existence of an æof the form

$$\sigma_n(x) \;=\; \arcsin(x) \;+\; \sum_{m=1} \frac{c_m(x)}{n^{2m}} \;,$$

i.e. an asymptotic expansion of arbitrary order and with the desired limit. ■
At first sight, this result seems to be only of theoretical importance, because if one would approximate the arcsin-function with the sequence $\{\sigma_n\}$ as defined in (1.30), he would have to evaluate this function and its inverse in each step. But fortunately it is possible, very much like in (1.18), to compute the subsequence $\{\sigma_{2^i}(x)\}$ for all $i \in \mathbb{N}_0$ recursively:

Theorem 1.10
For arbitrary $x \in [-1,1]$, define the sequence $\{y_i\}$ through $y_0 \;=\; x$ and for $i = 1,2,\ldots$:

$$y_i \;=\; \frac{\sqrt{2} \cdot y_{i-1}}{\sqrt{1+\sqrt{1-(y_{i-1}/2^{i-1})^2}}} \tag{1.31}$$

Then for all $i \in \mathbb{N}_0$:

$$y_i \;=\; y_i(x) \;=\; \sigma_{2^i}(x)$$

with σ defined in (1.30).
One easily recognizes the general principle standing behind this example; this motivates our next theorem, which is the central one of the present subsection.

Theorem 1.11 ([Walz1])
Let there be given a real interval I, of which the origin is an interior point, and consider some real function f, which maps I bijectively onto an interval J. Furthermore, assume that f possesses for all $x \in I$ the series expansion

$$f(x) \;=\; \sum_{\nu=1}^{\infty} a_\nu x^\nu$$

with $a_1 \neq 0$. Then the sequence of functions $\{\sigma_n(x)\}$, defined for all $n \in \mathbb{N}$ through

$$\sigma_n(x) \;:=\; n \cdot a_1 \cdot f^{-1}\left(\frac{f(x)}{n}\right), \tag{1.32}$$

possesses an asymptotic expansion of arbitrary order with limit $f(x)$.
Obviously, Theorem 1.11 allows a lot of modifications; we will indicate two of these in the following remarks.

Remark
1. The structure of the series expansion of f^{-1} carries over very closely to that of the resulting asymptotic expansion. If, for example, the series of f^{-1} contains only odd powers of y, then the asymptotic expansion of (1.32) contains only even powers of n (cf. the arcsin-example from above), a very desirable situation in extrapolation theory.
However, also in the general case it is possible to produce asymptotic expansions of this type, namely by defining

$$\tilde{\sigma}_n(x) = \frac{n \cdot a_1}{2} \cdot \left(f^{-1}\left(\frac{f(x)}{n}\right) - f^{-1}\left(\frac{f(x)}{-n}\right)\right). \tag{1.33}$$

2. A closer look into the proof of Theorem 1.11 shows that one could as well replace the function $f(x)$ in (1.32) by any other function $g(x)$ (and a_1 by $1/b_1$), and would still obtain an asymptotic expansion, in this case of course with limit $g(x)$. For some special cases this approach was proposed by Filippi [Filippi] and Rutishauser [Rutish].

However, this method has in general a serious drawback: As we shall see, the elements of the subsequence $\{\sigma_{2^i}(x)\}$ can in many cases be computed recursively, provided that the first one, $\sigma_1(x)$, is known. Now, with our approach this is easy, since always $\sigma_1(x) = a_1 x$, but in the other case one only has that

$$\sigma_1(x) \;=\; a_1 f^{-1}(g(x)) \;,$$

which can only in very special cases be computed excplicitly.
Let us continue with another example for Theorem 1.11. The function

$$f(x) \;:=\; \log(1+x) \;=\; \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j} x^j$$

satisfies the assumptions of the theorem on any interval $I = [-\alpha, \alpha]$ with $0 < \alpha < 1$, its inverse function being

$$f^{-1}(y) \;=\; \exp(y) - 1 \;.$$

Therefore the functions

$$\sigma_n(x) \;:=\; n \cdot \left(\exp\left(\frac{\log(1+x)}{n}\right) - 1\right)$$

possess the asymptotic expansion

$$\sigma_n(x) \;=\; \log(1+x) \;+\; \sum_{m=1} \frac{c_m(x)}{n^m} \;.$$

We remark that in this case *all* elements $\sigma_n(x)$ can be computed by elementary operations, since for all $n \in \mathbb{N}$ we have

$$\sigma_n(x) \;=\; n \cdot ((1+x)^{1/n} - 1),$$

a well-known formula for the numerical computation of the natural logarithm.

Finally, an application of the construction indicated in (1.33) leads us to the functions

$$\tilde{\sigma}_n(x) \;=\; \frac{n}{2}\cdot\Big((1+x)^{1/n}-(1+x)^{-1/n}\Big)\;,$$

which possess an expansion of the type

$$\tilde{\sigma}_n(x) \;=\; \log(1+x)\;+\;\sum_{m=1}\frac{c_{2m}(x)}{n^{2m}}\;.$$

1.2.5 Discretization Methods for Ordinary Differential Equations

Discretization methods for the numerical solution of differential equations establish one the most important disciplines in numerical analysis, where asymptotic expansions and extrapolation methods play a prominent role. In this section we give only a first impression of these methods; in particular, we concentrate on single-step methods for first order problems. Readers interested in multistep methods, higher order problems or more general topics as well as in the proofs of the following results are kindly referred to [Walz9].
We consider the initial value problem for a first order ordinary differential equation

$$y' = f(t,y)\,,\quad y(t_0) = y_0, \tag{1.34}$$

where f is assumed to be sufficiently smooth. Suppose we want to compute a numerical approximation of the value $y(x)$, where x is some real number. To do this, we use a one-step method, i.e. a numerical procedure of the form

$$y_{\nu+1} \;:=\; y_\nu + h\Phi(t_\nu, y_\nu, h) \tag{1.35}$$

for $\nu = 0,\dots,n-1$, with

$$h \;:=\; \frac{x-t_0}{n} \quad\text{and}\quad t_\nu = t_0 + \nu\cdot h, \tag{1.36}$$

and take y_n as an approximation for $y(x)$. Everywhere in this section, y_n (i.e., the index n) will denote the final result of a process like (1.35), while y_ν is intermediate value of this process; in other words, $n\cdot h$ is constant as n goes to infinity. The user-chosen number n is usually denoted as stepsize parameter, whereas we shall speak of h as the stepsize; the function Φ is the increment function of the one-step method (1.35).
We shall assume throughout that the increment function Φ and therefore also the numerical procedure (1.35) is sufficiently smooth and consistent with the problem (1.34), which can be expressed through the condition

$$\Phi(t,y,0) \;=\; f(t,y) \quad\text{for all}\;\;(t,y)\;.$$

In order to get some information on the global error $(y_n - y(x))$ of a method, it is reasonable to study first the so-called local error, i.e. that portion of the error that is brought in by going from ν to $(\nu+1)$ in (1.35). The precise definition of the term local error is by no means unique in the literature; we shall follow the approach given in [HNW] and define the term

$$l(t,h) \;:=\; y(t+h) - y(t) - h\Phi(t,y(t),h)$$

as the local error (function) of the method (1.35).

Using Taylor expansion, it can easily be shown that the local error of a consistent method is of order $O(h^2)$ at least.

Example 1.6
Consider the increment function $\Phi(t,y,h) := f(t,y)$, which defines Euler's method

$$y_{\nu+1} \; := \; y_\nu + h f(t_\nu, y_\nu)\,,$$

and apply it to the first order problem

$$y \; = \; y'\,, \quad y(0) = 1$$

with the solution $y(t) = \mathrm{e}^t$. The local error function is given by

$$l(t,h) \; = \; \mathrm{e}^t\,(\mathrm{e}^h - (1+h))\,,$$

and we see, using Taylor expansion and (1.36), that $l(t,h)$ possesses the asymptotic expansion

$$l(t,h) \; = \; \sum_{\mu=2} \frac{c_m(t)}{n^m}\,.$$

■

This behavior of the local error is typical for almost all one-step methods. The hope is now that the existence of an asymptotic expansion carries over from the local to the global error. In the present example, this is indeed true and can be proved directly, since after n steps with stepsize $h = x/n$ the approximating value y_n can be written in closed form by $y_n = (1 + x/n)^n$, which is already known to possess an asymptotic expansion.
Of course it cannot be expected in general that there is a closed-form representation of y_n. However, there is the following fundamental Theorem 1.12, which says that the existence of an asymptotic expansion of the local error always implies the existence of an asymptotic expansion of the global error. The first proof of this result, which was quite long and difficult (but remember that the first proof of an interesting result may be as ugly as it wants to be!), is due to Gragg [Gragg1, Gragg2]; the form of the statement as well as the proof below is due to Hairer and Lubich [HaLu]. In my opinion, it is the most beautiful and at the same time straightforward approach that is possible; therefore, in contrast to the remark at the beginning we present at least an outline of this proof.

Theorem 1.12 ([Gragg1], [Gragg2], [HaLu])
In addition to the assumptions above, suppose that the local error function of the one-step method (1.35) possesses an asymptotic expansion of order $M+1$ of the form

$$l(t,h) \; = \; \sum_{m=p+1}^{M+1} d_m(t) \cdot h^m \; + o(h^{M+1}) \qquad \textit{for } h \to 0\,, \tag{1.37}$$

where M is some integer greater than or equal to p.
Then the global error possesses the following asymptotic expansion of order M:

$$y_n \; = \; y(x) \; + \; \sum_{m=p}^{M} e_m(x) \cdot h^m \; + o(h^M) \qquad \textit{for } h \to 0\,. \tag{1.38}$$

Proof: The proof is by induction with respect to M, so let us start with $M = p$ and define a function e_p as the (unique) solution of the initial value problem

$$e'_p(t) \;=\; \frac{\partial}{\partial y} f(t,y(t))\, e_p(t) - d_{p+1}(t)\,, \quad e_p(t_0) = 0\,. \tag{1.39}$$

With this function e_p, we consider now a new increment function, say $\Phi^{(1)}$, defined by

$$\Phi^{(1)}(t,y(t),h) \;:=\; \Phi\big(t,y(t)+e_p(t)h^p,h\big) - \big(e_p(t+h)-e_p(t)\big)h^{p-1}\,, \tag{1.40}$$

and the hereby also defined one-step method

$$y^{(1)}_{\nu+1} \;:=\; y^{(1)}_\nu + h\Phi^{(1)}(t_\nu, y^{(1)}_\nu, h)\;,\; y^{(1)}_0 := y_0\,. \tag{1.41}$$

Expanding the local error of this method, say $l^{(1)}(t,h)$, into powers of h we obtain

$$\begin{aligned} l^{(1)}(t,h) \;&=\; y(t+h) - y(t) - h\Phi^{(1)}(t,y(t),h) \\ &=\; \left[d_{p+1}(t) - \frac{\partial}{\partial y}\Phi(t,y,0)e_p(t) + e'_p(t)\right] h^{p+1} + O(h^{p+2}), \end{aligned} \tag{1.42}$$

where we have used (1.37) and

$$\frac{\partial}{\partial y}\Phi(t,y,h) \;=\; \frac{\partial}{\partial y}\Phi(t,y,0) \;+\; O(h)$$

(remember that Φ was assumed to be sufficiently differentiable).
Since e_p is the solution of the initial value problem (1.39), we see, using

$$\frac{\partial}{\partial y}\Phi(t,y,0) \;=\; \frac{\partial}{\partial y} f(t,y)$$

that the h^{p+1}-term in (1.42) vanishes. Therefore, the local error $l^{(1)}(t,h)$ is of order $O(h^{p+2})$, and a standard result implies that the method defined by $\Phi^{(1)}$ converges and is of order $O(h^{p+1})$, i.e.

$$y^{(1)}_n - y(x) \;=\; O(h^{p+1}) = \; o(h^p)\,. \tag{1.43}$$

Comparing now equation (1.35) with (1.41) we see that (1.40) implies the relation

$$y^{(1)}_n \;=\; y_n - e_p(x)h^p\,.$$

Therefore, from (1.43),

$$y_n \;=\; y(x) + e_p(x)h^p + o(h^p)\,,$$

and the first term of the proposed æhas been determined.
If $M = p$, the proof is complete. Otherwise, we repeat the procedure from above, thus defining new increment functions $\Phi^{(2)}, \Phi^{(3)}, \ldots$, until the full asymptotic expansion in (1.38) is established.

As already pointed out in another context, a very attractive situation is given if the asymptotic expansion in (1.38) contains only even powers of h. If we ask for criteria, under which a one-step method possesses an h^2-expansion, the magic key word *symmetry* appears everywhere in the literature, i.e., symmetric methods possess h^2-expansions.
However, although this fact was known intuitively for quite a long time, its precise proof, and in particular an exact definition of the term symmetry in this context turned out to be a hard piece of work. The approach we are going to present is based mainly based on the work presented in [HNW].
Let us rewrite the one-step method (1.35) in the form

$$y(t+h) \;=\; y(t)+h\Phi(t,y(t),h)\;. \tag{1.44}$$

Definition 1.4
We call the one-step method (1.44) *symmetric,* if the increment function Φ keeps invariant after replacing h by $-h$ and then t by $t+h$, i.e. if we have formally

$$\Phi(t,y(t),h) \;=\; \Phi(t+h,y(t+h),-h)\;.$$

As a first example, we consider the trapezoidal rule

$$y_{\nu+1} \;=\; y_\nu + h\cdot\frac{f(t_\nu,y_\nu)+f(t_{\nu+1},y_{\nu+1})}{2} \tag{1.45}$$

and the *implicit midpoint rule*

$$y_{\nu+1} \;=\; y_\nu + hf\Big(\frac{t_\nu+t_{\nu+1}}{2},\frac{y_\nu+y_{\nu+1}}{2}\Big),$$

which are both easily seen to be symmetric.
The following Theorem 1.13 indicates why symmetry is such a desirable property in the context of asymptotic expansions and extrapolation methods.

Theorem 1.13
In addition to the assumptions of Theorem 1.12, let the one-step method under consideration be symmetric. Then the asymptotic expansion (1.38) of the global error is an h^2-expansion, i.e. it is of the form

$$y_n(x) \;=\; y(x) \;+\; \sum_{j=0}^{\widetilde{M}} e_{p+2j}(x)\cdot h^{p+2j} \;+o(h^{p+2\widetilde{M}}) \quad \textit{for } h\to 0. \tag{1.46}$$

Example 1.7
To give a first illustration of Theorem 1.13, let us continue our example from the beginning of this section, concerning the initial value problem

$$y \;=\; y'\;,\;\; y(0) \;=\; 1\;.$$

This time, we apply the trapezoidal rule (1.45), which gives us, after n steps with stepsize $h=x/n$, the final result

$$y_n \;=\; y_n(x) \;=\; \left(\frac{1+\frac{x}{2n}}{1-\frac{x}{2n}}\right)^n$$

in closed form.
Using again the functions $\sigma_n^e(x) = (1+\frac{x}{n})^n$ from above, we may also write

$$y_n(x) \;=\; \sigma_n^e(x/2)\cdot\sigma_{-n}^e(x/2)\,,$$

and from Theorem 1.4 it follows that $y_n(x)$ possesses the asymptotic expansion

$$y_n(x) = \left(\mathrm{e}^{\frac{x}{2}} + \sum_{\mu=1} \frac{c_\mu(\frac{x}{2})}{n^\mu}\right)\cdot\left(\mathrm{e}^{\frac{x}{2}} + \sum_{\mu=1} \frac{(-1)^\mu c_\mu(\frac{x}{2})}{n^\mu}\right) = \mathrm{e}^x \;+\; \sum_{\mu=1} \frac{d_\mu(x)}{n^\mu} \qquad (1.47)$$

with certain coefficient functions d_μ. Moreover, since $y_n(x) = y_{-n}(x)$ for all n and x, in (1.47) all d_μ with odd index must vanish, and we have finally proved that

$$y_n(x) \;=\; \mathrm{e}^x \;+\; \sum_{j=0} \frac{d_{2+2j}(x)}{n^{2+2j}}\,,$$

in accordance with Theorem 1.13. ■
We now turn shortly to another class of interesting one-step methods, which has been introduced and investigated in the last years; all methods in this class enjoy the property of being symmetric and therefore lead to h^2-expansions.
Let us start with the classical trapezoidal rule (cf. (1.45)), which we write now in the form

$$y_{\nu+1} \;=\; y_\nu + h\Psi^T(t_\nu,t_{\nu+1},y_\nu,y_{\nu+1},h)$$

with the increment function

$$\Psi^T := \Psi^T(t_\nu,t_{\nu+1},y_\nu,y_{\nu+1},h) := \frac{f(t_\nu,y_\nu)+f(t_{\nu+1},y_{\nu+1})}{2} \qquad (1.48)$$

This method was already recognized to be symmetric. The idea is now to replace the Arithmetic mean on the right-hand side of (1.48) by other – in general nonlinear – means, which gave the resulting one-step methods the name generalized trapezoidal rules. We consider the following types of means resp. increment functions:

$$\begin{aligned}
\Psi^G &:= \sqrt{f_\nu f_{\nu+1}} && \text{(Geometric)}\,,\\
\Psi^H &:= \frac{2f_\nu f_{\nu+1}}{f_\nu + f_{\nu+1}} && \text{(Harmonic)}\,,\\
\Psi^L &:= \frac{f_{\nu+1}-f_\nu}{\log(f_{\nu+1}/f_\nu)} && \text{(Logarithmic)}\,,\\
\Psi^* &:= \frac{f_\nu^2 + f_{\nu+1}^2}{f_\nu + f_{\nu+1}} && \text{(Contra-Harmonic)}\,.
\end{aligned}$$

Here we have used the abbreviations $f_\nu := f(t_\nu,y_\nu)$ and $f_{\nu+1} := f(t_{\nu+1},y_{\nu+1})$. Of course, in certain cases some additional assumptions on the f_ν's (e.g. positivity) have to be imposed, which we will always do in the following. The behavior of these one-step methods has been studied extensively in a series of papers by Evans and Sanugi [EvSa1], [EvSa2] and Evans and Walz [EvWa]. The main result concerning asymptotic expansions of these investigations is summarized in the next theorem; it turns out that each of these methods is of order 2 and possesses an h^2-expansion.

Theorem 1.14 ([EvWa])
Let Ψ denote an arbitrary one of the increment functions defined above, and consider the hereby defined one-step method

$$y_{\nu+1} \;=\; y_\nu + h\Psi(t_\nu, t_{\nu+1}, y_\nu, y_{\nu+1}, h)\,, \quad \nu = 0, \ldots, n-1,$$

with $h = (x - t_0)/n$ and $t_\nu = t_0 + \nu h$ for $\nu = 1, \ldots, n$. Then the global error of this method possesses an asymptotic expansion of the form

$$y_n(x) \;=\; y(x) + \sum_{m=1}^{M} c_{2m}(x) \cdot h^{2m} \; + o(h^{2M}) \qquad \textit{for } h \to 0\,.$$

The order M of this expansion depends on the smoothness properties of f resp. Ψ.
For numerical examples we refer again to the original paper [EvWa].

2 The matrix exponential

In this chapter we take a closer look onto the so-called matrix exponential function, which is a direct generalization of the real exponential function to the case of square matrices. Consequently, we will apply the generaliziation of the algorithm considered in section 1.2.2 to the matrix case, thus obtaining new numerical results.
Let us start with the precise definition of the terms under consideration.

2.1 Definition and basic properties

In this section we will define the matrix exponential as well as other matrix functions and have a look onto their fundamental properties.

2.1.1 The matrix exponential

In the theory of differential equations systems, the *matrix exponential (function)* $\exp(A)$ plays a very important role. The matrix exponential is the natural generalization of the well-known real exponential function

$$\exp(x) = \mathrm{e}^x \quad \text{for } x \in \mathbb{R}. \tag{2.1}$$

But how should this generalization work? Clearly, terms like e^A for a $(m \times m)$-matrix A make no sense.
So, the usual definition auf the matrix exponential is by applying the Taylor series of $\exp(x)$ to the matrix A in an appropriate way. The exact definition is as follows:

Definition 2.1
Let A be a square matrix, say $A \in \mathbb{R}^{m\times m}$. Then the matrix exponential of A is defined as

$$\exp(A) = \sum_{i=0}^{\infty} \frac{1}{i!} A^i, \tag{2.2}$$

where A^i denotes the i-fold multiplication of A with itself, and $A^0 = I$, the unit matrix
We want to give a first example for this. Since summation up to infinity is quite time-consuming, we use a matrix N which is nilpotent, i.e., N^k for some k is the zero matrix.

Example 2.1
Let

$$N = \begin{pmatrix} 0 & -1 & 2 \\ 0 & 0 & 3 \\ 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^{3\times 3}$$

Then

$$N^2 = \begin{pmatrix} 0 & 0 & -3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \; N^3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and therefore

$$N^i = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{for all } i \geq 3.$$

Thus the infinite series in Definition 2.1 reduces to a finite sum and yields

$$\exp(N) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & -1 & 2 \\ 0 & 0 & 3 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0 & 0 & -3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -1 & \frac{1}{2} \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{pmatrix}$$

■

Remark
Of course not all matrices in the world are nilpotent, but it can be shown that the series (2.2) converges für each matrix $A \in \mathbb{R}^{m \times m}$. Therefore, $\exp(A)$ is well-defined for all A.

Let us now collect some properties of the matrix exponential. For proofs and further examples see e.g. [Haber], [Higham] and the references therein.
The first result says that the computation of the matrix exponential for a diagonal matrix reduces to the computation of the usual real exponential function.

Theorem 2.1
Let D be a diagonal matrix, say

$$D = \begin{pmatrix} d_1 & 0 & 0 & \cdots & 0 \\ 0 & d_2 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & d_n \end{pmatrix}$$

Then

$$\exp(D) = \begin{pmatrix} \exp(d_1) & 0 & 0 & \cdots & 0 \\ 0 & \exp(d_2) & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & \exp(d_n) \end{pmatrix}$$

Proof: This comes directly from the definition, using the fact that

$$D^i = \begin{pmatrix} d_1^i & 0 & 0 & \cdots & 0 \\ 0 & d_2^i & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & d_n^i \end{pmatrix}$$

for all integers i. □

The following theorem says that the matrix exponential shares some important properties of the real exponential function:

Theorem 2.2
The matrix exponential has - between others - the following properties:
1. It is

$$\exp(0) = I,$$

where $\mathbf{0}$ *denotes the zero matrix.*
2. For each square matrix A*, it is*

$$\exp(A)^{-1} = \exp(-A). \tag{2.3}$$

In particular, $\exp(A)$ *is nonsingular.*
3. If x *denotes a real variable, then*

$$\frac{d}{dx}\exp(Ax) = A\exp(Ax). \tag{2.4}$$

Proof: The first statement comes directly from the definition.
To prove the second one, we first observe that

$$I = \exp(0) = \exp(A - A). \tag{2.5}$$

To complete the proof we need the fact that

$$\exp(A - A) = \exp(A) \cdot \exp(-A)$$

as in the real case. And this is in fact true, as it will turn out in Theorem 2.3.
Finally, the proof of the third statement is straightforward as follows:

$$\begin{aligned} \frac{d}{dx}\exp(Ax) &= \frac{d}{dx}\left(I + Ax + \frac{1}{2}A^2x^2 + \frac{1}{3!}A^3x^3 + \cdots\right) \\ &= A + A^2x + \frac{1}{2!}A^3x^2 + \cdots \\ &= A\exp(Ax). \end{aligned}$$

□

Let us look at a short example for the second statement:

Example 2.2
We use the matrix N from Example 2.1. Then

$$-N = \begin{pmatrix} 0 & 1 & -2 \\ 0 & 0 & -3 \\ 0 & 0 & 0 \end{pmatrix},$$

and, omitting intermediate calculations,

$$\exp(-N) = \begin{pmatrix} 1 & 1 & -\frac{7}{2} \\ 0 & 1 & -3 \\ 0 & 0 & 1 \end{pmatrix}.$$

So indeed

$$\exp(N)\cdot\exp(-N) = \begin{pmatrix} 1 & -1 & \frac{1}{2} \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 & -\frac{7}{2} \\ 0 & 1 & -3 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

as predicted. ■

A very attractive property of the real exponential function ist that $\exp(x+y) = \exp(x)\cdot\exp(y)$ holds for all numbers x and y. In the matrix case, this is true under an additional assumption.

Theorem 2.3
If two matrices A and B satisfy

$$A\cdot B = B\cdot A, \tag{2.6}$$

then

$$\exp(A+B) = \exp(A)\cdot\exp(B) = \exp(B)\cdot\exp(A). \tag{2.7}$$

In particular,

$$I = \exp(A-A) = \exp(A)\cdot\exp(-A) = \exp(-A)\cdot\exp(A)$$

for each matrix A.

The proof can be done strightforward, using the Definition 2.1.

2.1.2 Other matrix functions

The idea of taking the series expansion of a real function in oder to define their matrix counterpart can be transfered to other matrix functions in an obvious way. The proof of the following theorem can be found e.g. in [Stickel].

Theorem 2.4
Let, for some complex number a and a real number $r>0$, $K_r(a)$ denote the open disk

$$K_r(a) = \{z\in\mathbb{C}; |z-a|<r\}.$$

Furthermore, let $f(z)$ be a scalar function which possesses for all $z\in K_r(a)$ a series representation of the form

$$f(z) = \sum_{i=0}^{\infty} c_i(z-a)^i.$$

Then for each quadratic matrix A, whose eigenvalues all lie in $K_r(a)$, the matrix function

$$f(A) = \sum_{i=0}^{\infty} c_i(A-aI)^i$$

is well-defined.

Therefore, functions as $\sin(A)$, $\cos(A)$ and of course $\exp(A)$ are well-defined for all quadratic matrices A. But also rather funny things like $\arcsin(A)$ may be defined (see [Walz2]).

Furthermore, we may define the matrix logarithm as follows:

Definition 2.2
For a quadratic matrix A, the (natural) matrix logarithm is defined as

$$\log(A) = \sum_{i=1}^{\infty} \frac{(-1)^{i+1}}{i} \cdot (A-I)^i$$

whenever this series converges. This is in particular the fact, if all eigenvalues of A lie in $K_1(1)$, or, if the matrix $A-I$ is nilpotent.

Example 2.3
Let

$$A = \begin{pmatrix} 1 & -1 & \frac{1}{2} \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then

$$A - I = \begin{pmatrix} 0 & -1 & \frac{1}{2} \\ 0 & 0 & 3 \\ 0 & 0 & 0 \end{pmatrix}$$

and

$$(A-I)^2 = \begin{pmatrix} 0 & 0 & -3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ (A-I)^3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

Thus, $(A-I)$ is nilpotent, and we have

$$\log(A) = \begin{pmatrix} 0 & -1 & \frac{1}{2} \\ 0 & 0 & 3 \\ 0 & 0 & 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 0 & 0 & -3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 2 \\ 0 & 0 & 3 \\ 0 & 0 & 0 \end{pmatrix}$$

Note that this is again the matrix N from Example 2.1, thus we have here

$$\log(\exp(N)) = \log(A) = N$$

as expected. ■

2.2 Numerical computation of the matrix exponential

2.2.1 Preliminaries

We now come back to the matrix exponential, in particular to the question, how this function can be computed numerically. Of course, it is possible to do this by evaluating partial sums of the series in (2.2). But it turns out that the convergence of this series is much too slow to give a satisfactory result in finite time.
There are also some other numerical methods, a survey of which can be found e.g. in [MoLo] or [Higham] and the references therein, an additional method was proposed by Stickel ([Stickel]). Furthermore, in [Walz2], [Walz3], an at that time new method using extrapolation was proposed, but due to limited computer capacities not numerically tested in a sufficient way. It is the purpose of this

chapter to give a short review of the method and in particular to provide the results of extensive numerical tests.

2.2.2 The Method

The follouing statement, which will turn out to be an important step in our method, is well-known since many years.

Theorem 2.5
Let A be an arbitrary quadratic matrix, and define for, $n \in \mathbb{N}$, the sequence of matrices

$$S_n(A) = \left(I + \frac{1}{n}A\right)^n. \tag{2.8}$$

Then

$$\lim_{n\to\infty} S_n(A) = \exp(A). \tag{2.9}$$

For practical computations the convergence of the sequence $S_n(A)$ is too slow, but the asssertion in (2.9) can be sharpened significantly:

Theorem 2.6 ([Walz2])
The sequence of matrices $S_n(A)$, defined in (2.8), possesses an asymptotic expansion of arbitrary order with limit $\exp(A)$, i.e.:

$$S_n(A) = \exp(A) + \sum_{j=1} \frac{1}{n^j} C_j(A).$$

As pointed out in chapter 1, the existence of an asymptotic expansion justifies the application of an extrapolation process to the sequence $S_n(A)$, in order to accelerate the convergence signifantly. This leads to the following algorithm for the numerical computation of $\exp(A)$ for given quadratic matrix A (see [Walz2], [Walz3]). Note that extrapolation is a completely linear process, such that it can be passed from numbers to matrices without problems.

Algorithm for the numerical computation of the matrix exponential

1. Choose a maximal Index k_{max}
2. Compute

$$Y_i^{(0)} = S_{2^i}(A)$$

for $i = 0, 1, \ldots, k_{max}$. This can be done by iterated squaring.
3. Compute

$$Y_i^{(k)} = Y_{i+1}^{(k-1)} + \frac{1}{2^k - 1} \cdot (Y_{i+1}^{(k-1)} - Y_i^{(k-1)})$$

for $k = 1, 2, \ldots, k_{max}$ and $i = 0, 1, \ldots, k_{max} - k$.
4. Take $Y_0^{(k_{max})}$ as an approximation of $\exp(A)$.

Remark

Step 3 can also be performed in the equivalent form

$$Y_i^{(k)} = \frac{1}{2^k - 1} \cdot (2^k Y_{i+1}^{(k-1)} - Y_i^{(k-1)}).$$

The justification of the statement in step 4 is given in the following theorem.

Theorem 2.7 ([Walz2])
The sequence of matrices $Y_i^{(k)}$ possesses an asymptotic expansion of arbitrary order of the form

$$Y_i^{(k)} = \exp(A) + \sum_{j=k+1} \frac{1}{2^{ij}} \tilde{C}_j(A),$$

i.e., for each fixed k, the sequence $\{Y_i^{(k)}\}$ converges to $\exp(A)$ with an error of order $O(2^{-i(k+1)})$.
In the next section we give an outline of the results of extensive numerical tests in order to illustrate the correctness and efficiency of the proposed algorithm.

2.2.3 Numerical Results

Example 2.4
As a first test and more or less just for fun we tried the nilpotent matrix already considered in Example 2.1. As expected (or should I say: hoped), the algorithm computed the exact result

$$\begin{pmatrix} 1.0 & -1.0 & 0.5 \\ 0.0 & 1.0 & 3.0 \\ 0.0 & 0.0 & 1.0 \end{pmatrix}$$

already with $k_{max} = 1$. ■
The next two examples are more serious, but still the exact result is known and can therefore used for control.

Example 2.5
Consider a (2×2)-matrix of the form

$$B = \begin{pmatrix} 0 & b \\ -b & 0 \end{pmatrix}$$

It can easily be shown by induction that for all $i \in \mathbb{N}_0$

$$B^{4i} = \begin{pmatrix} b^{4i} & 0 \\ 0 & b^{4i} \end{pmatrix}$$

$$B^{4i+1} = \begin{pmatrix} 0 & b^{4i+1} \\ -b^{4i+1} & 0 \end{pmatrix}$$

$$B^{4i+2} = \begin{pmatrix} -b^{4i+2} & 0 \\ 0 & -b^{4i+2} \end{pmatrix}$$

$$B^{4i+3} = \begin{pmatrix} 0 & -b^{4i+3} \\ b^{4i+3} & 0 \end{pmatrix}$$

and so

$$\exp(B) = \begin{pmatrix} \cos(b) & \sin(b) \\ -\sin(b) & \cos(b) \end{pmatrix}$$

If we choose, for example, $b = 0.8$, thus

$$B = \begin{pmatrix} 0 & 0.8 \\ -0.8 & 0 \end{pmatrix}, \tag{2.10}$$

we obtain - with an 8-digit-accuracy -

$$\exp(B) = \begin{pmatrix} 0.69670670 & 0.71735609 \\ -0.71735609 & 0.69670670 \end{pmatrix}$$

In approximatig this we used the proposed algorithm with $k_{max} = 4$ as a first attempt. The result was

$$Y_0^{(4)} = \begin{pmatrix} 0.69674685 & 0.71737079 \\ -0.71737079 & 0.69674685 \end{pmatrix}, \tag{2.11}$$

which is correct up to four digits.
Setting $k_{max} = 6$ alredy gives

$$Y_0^{(6)} = \begin{pmatrix} 0.69670670 & 0.71735609 \\ -0.71735609 & 0.69670670 \end{pmatrix}, \tag{2.12}$$

which is correct in all shown digits. ■

Example 2.6
As pointed out in Theorem 2.1, the matrix exponential of a diagonal matrix is easy to compute. We will use this fact to give another verification of the proposed algorithm. To save space we will use the notation

$$\mathrm{diag}(d_1, d_2, \dots, d_n) \quad \text{for} \quad \begin{pmatrix} d_1 & 0 & 0 & \cdots & 0 \\ 0 & d_2 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & d_n \end{pmatrix} \tag{2.13}$$

Using this notation, we will compute numerically

$$\begin{aligned} &\exp(\ \mathrm{diag}(-1, 0.5, 1, 2)) \\ &\quad = \ \mathrm{diag}(\exp(-1), \exp(0.5), \exp(1), \exp(-2)) \\ &\quad = \ \mathrm{diag}(0.3678794411, 1.6487212707, 2.7182818284, 0.1353352832). \end{aligned}$$

Since the presentation of all intermediate results in form of a Romberg table is rather space-consuming, we just show the upmost entries of each column, i.e., the values $Y_0^{(k)}$, $k = 0, \dots, k_{max}$. Choosing $k_{max} = 8$ we obtained the results

$$\begin{aligned} Y_0^{(0)} &= \ \mathrm{diag}(0.0000000000, 1.5000000000, 2.0000000000, -1.0000000000) \\ Y_0^{(1)} &= \ \mathrm{diag}(0.5000000000, 1.6250000000, 2.5000000000, \quad 1.0000000000) \\ Y_0^{(2)} &= \ \mathrm{diag}(0.3437500000, 1.6464843750, 2.6770833333, -0.1666666666) \\ Y_0^{(3)} &= \ \mathrm{diag}(0.3701057434, 1.6486054382, 2.7138789948, \quad 0.1860584077) \\ Y_0^{(4)} &= \ \mathrm{diag}(0.3677749219, 1.6487181048, 2.7180298346, \quad 0.1310866624) \\ Y_0^{(5)} &= \ \mathrm{diag}(0.3678819473, 1.6487212260, 2.7182743438, \quad 0.1355159712) \\ Y_0^{(6)} &= \ \mathrm{diag}(0.3678794104, 1.6487212703, 2.7182817150, \quad 0.1353313529) \\ Y_0^{(7)} &= \ \mathrm{diag}(0.3678794413, 1.6487212706, 2.7182818275, \quad 0.1353353270) \\ Y_0^{(8)} &= \ \mathrm{diag}(0.3678794411, 1.6487212707, 2.7182818284, \quad 0.1353352829) \end{aligned}$$

which should be compared with the exact values above. ■
Let us now look at some examples, where the results can not be computed explicitly, and therefore there is essential need for numerical methods.

Example 2.7
First we give an illustration of formula $\exp(A)^{-1} = \exp(-A)$, stated in Theorem 2.3. We chose the matrix

$$A = \begin{pmatrix} 1.0 & -2.0 & 0.0 \\ 3.0 & 0.0 & 1.0 \\ -1.0 & -1.0 & 2.0 \end{pmatrix},$$

hence

$$-A = \begin{pmatrix} -1.0 & 2.0 & 0.0 \\ -3.0 & 0.0 & -1.0 \\ 1.0 & 1.0 & -2.0 \end{pmatrix}$$

Using $k_{max} = 12$, our algorithm computed the results

$$\exp(A) =$$
$$\begin{pmatrix} -0.04882097901021 & -0.78283329067919 & -1.88174352465658 \\ 0.23337817369046 & -1.38110938667791 & 1.33228840766776 \\ -5.09577545698056 & 0.54945511698858 & 6.92869800262720 \end{pmatrix}$$

and

$$\exp(-A) =$$
$$\begin{pmatrix} -0.51287264916926 & 0.21856930515847 & -0.18131720239588 \\ -0.41851255893563 & -0.49424659778797 & -0.01862605138129 \\ -0.34400835341044 & 0.19994325377715 & 0.01245290663710 \end{pmatrix}$$

And indeed, as you may verify, we have here $\exp(A) \cdot \exp(-A) = I$. ■

Example 2.8
Believe it or not, but we now treat a (2×2)-matrix, namely

$$M = \begin{pmatrix} -49 & 24 \\ -64 & 31 \end{pmatrix}$$

Although it looks quite harmless, in the context of computing the matrix exponential it is by far not. In their paper [MoLo] the authors used the Taylor series approach and obtained, using 6-digit accuracy,

$$\begin{pmatrix} -22.25880 & -1.432736 \\ -61.49931 & -3.474280 \end{pmatrix} \tag{2.14}$$

as an „approximation“ of $\exp(M)$. But the true result is

$$\exp(M) = \begin{pmatrix} -0.735759 & 0.551819 \\ -1.471517 & 1.103638 \end{pmatrix} \tag{2.15}$$

and has obviously nothing in common with (2.14). This of course due to rounding errors, but using the same accuracy our algorithm still produced three exact decimals (with $k_{max} = 9$).
If we use higher accuracy and $k_{max} = 10$, we get the exact result from above.
Interesting is here the way „in between“. To illustrate what ist meant here, saving at the same time some pages of text, we show similar as in Example 2.6, the upmost entries of the Romberg table, i.e., the values $Y_0^{(k)}$, $k = 0, \ldots, 10$.
See what happened:

$$Y_0^{(0)} = \begin{pmatrix} -48.000000 & 24.000000 \\ -64.000000 & 32.000000 \end{pmatrix}$$
$$Y_0^{(1)} = \begin{pmatrix} 384.500000 & -192.000000 \\ 512.000000 & -255.500000 \end{pmatrix}$$
$$Y_0^{(2)} = \begin{pmatrix} 538.343750 & -269.000000 \\ 717.333333 & -358.322916 \end{pmatrix}$$
$$Y_0^{(3)} = \begin{pmatrix} -755.027145 & 377.698625 \\ -1007.196335 & 503.968273 \end{pmatrix}$$
$$Y_0^{(4)} = \begin{pmatrix} 257.092456 & -128.362340 \\ 342.299574 & -170.782012 \end{pmatrix}$$
$$Y_0^{(5)} = \begin{pmatrix} -34.341374 & 17.354628 \\ -46.279008 & 23.507386 \end{pmatrix}$$
$$Y_0^{(6)} = \begin{pmatrix} 0.945957 & -0.289038 \\ 0.770770 & -0.017505 \end{pmatrix}$$
$$Y_0^{(7)} = \begin{pmatrix} -0.752138 & 0.560009 \\ -1.493357 & 1.114558 \end{pmatrix}$$
$$Y_0^{(8)} = \begin{pmatrix} -0.736714 & 0.552297 \\ -1.472792 & 1.104275 \end{pmatrix}$$

$$Y_0^{(9)} = \begin{pmatrix} -0.735732 & 0.551805 \\ -1.471481 & 1.103620 \end{pmatrix}$$
$$Y_0^{(10)} = \begin{pmatrix} -0.735759 & 0.551819 \\ -1.471517 & 1.103638 \end{pmatrix}$$

So, in the first steps, the results seem to „explode“, but very soon they converge to a rather satisfactory final result. ■

Let us finish the paper as we started it, namely showing a complete Romberg table:

Example 2.9

We calculated the exponential of the matrix

$$B = \begin{pmatrix} -2.0 & 0.0 & 4.0 \\ 4.0 & -2.0 & -2.0 \\ 0.0 & 0.0 & 1.0 \end{pmatrix},$$

and obtained, using $k_{max} = 9$, the result

$$\exp(B) = \begin{pmatrix} 0.135335283 & 0.000000000 & 3.443928726 \\ 0.541341132 & 0.135335283 & 2.148152428 \\ 0.000000000 & 0.000000000 & 2.718281828 \end{pmatrix}$$

which is correct in all digits shown.
Now, what about the intermediate steps? Of course, displaying the Romberg table with (3×3)-matrices as entries is too space-consuming, so we show the Romberg table of the computation of one specific element and chose – for no deeper reason – the one in the first column and second line. Since this is still to wide to show it on this page, I splitted it into two parts, to be seen in Tables 2.1 and 2.2.

4.000000000				
	−4.00000000			
0.000000000		2.666666666		
	1.000000000		0.103422619	
0.500000000		0.423828125		0.584478654
	0.567871093		0.554412652	
0.533935546		0.538089586		0.540650059
	0.545534963		0.541510221	
0.539735254		0.541082641		0.541336950
	0.542195722		0.541347779	
0.540965488		0.541314637		0.541341051
	0.541534908		0.541341472	
0.541250198		0.541338117		0.541341130
	0.541387315		0.541341152	
0.541318757		0.541340772		0.541341132
	0.541352408		0.541341134	
0.541335582		0.541341088		
	0.541343918			
0.541339750				

Table 2.1: Romberg table Part 1

0.539236233				
	0.541392804			
0.541359108		0.541340490		
	0.541340899		0.541341136	
0.541341183		0.541341134		0.541341132
	0.541341132		0.541341132	
0.541341133		0.541341132		
	0.541341132			
0.541341132				

Table 2.2: Romberg table Part 2

It is quite obvious that the results in each single column converge to to the correct result 0.541341132, but the rate of convergence invreases from column to column, as predicted.
Bounds for the remeinig errors and consequentlx stoppimg rules for the algorithm were given in [Walz5], see also [Walz9]. ■

3 Concluding Remarks

In the situation of real functions, it is well-known that the sequences

$$s_n^1(x) = \frac{1}{2}\left(\left(1+\frac{x}{n}\right)^n + \left(1-\frac{x}{n}\right)^{-n}\right) \tag{3.1}$$

as well as

$$s_n^2(x) = \left(\frac{1+\frac{x}{2n}}{1-\frac{x}{2n}}\right)^n = \left(1+\frac{x}{2n}\right)^n \cdot \left(1-\frac{x}{2n}\right)^{-n} \tag{3.2}$$

both possess an asymptotic expansion of the form

$$s_n^i(x) = \exp(x) + \sum_{m=1} \frac{C_m^i(x)}{n^{2m}}$$

i.e., expansions of arbitrary order with limit $\exp(x)$ and with respect to the set of exponents $\{2,4,6,\ldots\}$. This means that the extrapolation process, applied to these sequences, will converge faster than the one applied to $(1+\frac{x}{n})^n$. Therefore it is tempting to do the same with the matrix functions, i.e., to consider the sequences $S_n^i(A)$, defined by

$$S_n^1(A) = \frac{1}{2}\left(\left(I+\frac{1}{n}A\right)^n + \left(I-\frac{1}{n}A\right)^{-n}\right) \tag{3.3}$$

and

$$S_n^2(A) = \left(I+\frac{1}{2n}A\right)^n \cdot \left(I-\frac{1}{2n}A\right)^{-n} \tag{3.4}$$

This indeed does work in theory, but in practice the calculations in (3.3) as well as in (3.4) require the computation of matrix inverses, which is numerically, say, challenging. Therefore we do not seriously suggest this approach.

Similar is true for the numerial calulation of other matrix functions like the matrix logarithm introduced in Definition 2.2, Here, a good approximation is provided by

$$L_n(A) = n \cdot \left((I+A)^{1/n} - I\right). \tag{3.5}$$

More precisely, the asymptotic expansion

$$L_n(A) = \log(A) + \sum_{m=1} \frac{1}{n^m} \cdot B_m(A)$$

is valid. But here, in practice the n-th roots of a matrix must be calculated, which is even much more challenging than the computation of the inverse.

But since we do not want to finish this paper with a collection of negative assertions, we finally cite a result found and proved in [Walz1], see also [Walz4]:

Theorem 3.1
Suppose that A is a square matrix whose eigenvalues all lie in $K_1(0)$. Define

$$Y_0 = A^2,$$

and, for $i = 1, 2, \ldots$:

$$Y_i = 2Y_{i-1}\left(I + \sqrt{I - \frac{1}{4^{i-1}}Y_{i-1}}\right)$$

Then

$$Y_i = Y_i(A) = S_{2^i}(A)$$

where

$$S_n(A) = \arcsin^2(A) + \sum_{m=1} \frac{1}{n^{2m}} C_m(A).$$

Note that here only the calculation of square roots is necessary; methods for this can be found e.g. in [Stickel].

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