

The History of Extrapolation Methods in Numerical Analysis

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Summary: We give a short survey over the history of linear extrapolation methods, which are nowadays an important tool in numerical analysis.

Starting with a fundamental idea of Archimedes in 250 BC, we first sketch the development of these methods during the centuries until the famous paper of Richardson/Gaunt from [1927]. Then we shall have a deeper look into the very nice book of Kommerell [1936], which is not very well known today, although in it already the famous method of Romberg from [Romberg 1955] is anticipated. We will analyze this part of Kommerell's book in some detail.

Finally, the development since 1955 will be indicated, including a short list of researchers, who are nowadays the outstanding figures in the theory of extrapolation methods.

Zusammenfassung: Wir geben einen kurzen Überblick über die Geschichte von (linearen) Extrapolationsverfahren, die heutzutage ein sehr wichtiges Instrument innerhalb der Numerischen Mathematik sind.

Beginnend mit einer grundlegenden Idee von Archimedes aus dem Jahre 250 v.Chr. skizzieren wir zunächst die Entwicklung dieser Methoden über die Jahrhunderte hinweg bis zur berühmten Arbeit von Richardson/Gaunt [1927]. Danach werden wir einen etwas tieferen Blick in das sehr schöne Buch von Kommerell [1936] werfen, das offenbar weitgehend unbekannt ist, obwohl in ihm bereits das berühmte Romberg-Verfahren aus [Romberg 1955] vorweggenommen ist. Den diesbezüglichen Teil von Kommerell's Buch werden wir etwas detaillierter analysieren.

Abschließend wird die Entwicklung seit 1955 angedeutet, inclusive einer kleinen Liste von Forschern, die heute die herausragenden Persönlichkeiten auf dem Gebiet der Extrapolationsverfahren sind.

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1. Introduction

In this little note we want to study the historical roots of so-called (*linear*) *extrapolation methods*, which are nowadays frequently used in numerical analysis. For reasons we are going to explain later on, such methods are often called *Richardson extrapolation* or *Romberg type methods*. As we shall see, there could have been better choices for their names, but of course this is not the only time that theories or methods are named after their rediscoverers instead of the original discoverers.

We would like to point out that there do already exist a few studies on the history of extrapolation methods, e.g. the papers of H.Engels [1979] and J.Dutka [1984]; also the excellent survey paper of D.C.Joyce [1971] contains many historical references. However, all these papers enlight only a part of the story, (in particular the connection with asymptotic expansions in not worked out well), so we shall try to supply some more information in order to give a complete survey of the history, partially based of course on authors like the ones quoted above. In particular, we will have a deeper look into the book of K.Kommerell [1936], which seems not to be very well-known, although in it already the main idea of “Romberg’s principle” can be found.

First we give a (short) definition of the terms “asymptotic expansion” and “extrapolation method”; more information on this topic can be found in many places, we refer to Brezinski/Redivo Zaglia [1991], Joyce [1971], Walz [1987], [1992] and the references therein.

Let there be given a family of complex numbers $T(h)$, where h is a real non-negative parameter, and assume that there are numbers G, c_1, \dots, c_m and $\rho_1, \dots, \rho_{m+1}$ with

$$0 < \operatorname{Re}\rho_1 < \operatorname{Re}\rho_2 < \dots < \operatorname{Re}\rho_{m+1} ,$$

not depending on h , such that a relation of the form

$$T(h) = G + \sum_{\nu=1}^m c_\nu h^{\rho_\nu} + O(h^{\operatorname{Re}\rho_{m+1}}) \quad \text{for } h \rightarrow 0 \quad (1.1)$$

is valid. Then the family $\{T(h)\}$ is said to possess an *asymptotic expansion (AE)* for $h \rightarrow 0$.

It is tacitly assumed that the value $T(0) = G$, in which we are interested, cannot be computed explicitly, while the values $T(h)$ for $h > 0$ can. This is the situation which

occurs quite frequently in numerical analysis. An obvious way to solve this problem at least approximately is of course to compute the values of $T(h)$ for some small values of h and to take these as approximations to G . However, in most applications, the convergence of the sequence $\{T(h)\}$ for $h \rightarrow 0$ is rather slow, so one is interested in methods for the acceleration of convergence. Due to the special structure (1.1), it is possible here to apply (linear) extrapolation methods to reach this goal. The most widespread type of such an extrapolation method is given in the following lemma.

Lemma 1: *Let the family $\{T(h)\}$ possess an asymptotic expansion of the type (1.1). Then choose a number h_0 and define the sequences $\{T_i^{(k)}\}_{i,k \in \mathbb{N}}$ through*

$$\left. \begin{aligned} T_i^{(0)} &= T(h_0/2^i) \quad \text{for } i = 0, 1, \dots \\ T_i^{(k)} &= T_{i+1}^{(k-1)} + \frac{1}{2^{\rho_k} - 1} \cdot (T_{i+1}^{(k-1)} - T_i^{(k-1)}) \quad \left\{ \begin{array}{l} k = 1, 2, \dots \\ i = 0, 1, \dots \end{array} \right. \end{aligned} \right\} \quad (1.2)$$

Then the sequences $\{T_i^{(k)}\}_{i \in \mathbb{N}}$ possess the asymptotic expansion

$$T_i^{(k)} = G + \sum_{\mu=k+1}^m c_\mu^{(k)} \cdot 2^{-i \cdot \rho_\mu} + O(2^{-i \rho_{m+1}}) \quad \text{for } i \rightarrow \infty \quad (1.3)$$

with certain coefficients $c_\mu^{(k)}$, which are not depending on i .

Roughly spoken, Lemma 1 says that, for each k , the sequence $\{T_i^{(k)}\}$ converges faster to the limit value G than $\{T_i^{(k-1)}\}$, as i tends to infinity. Therefore, the iterative process (1.2) is a special case of a convergence acceleration method. It is called (linear) extrapolation and is usually connected with the names of Richardson and Romberg. As we shall see in the next sections, there are quite a lot more people to whom numerical analysis is indebted in this connection.

2. From Archimedes to Richardson

In this section we shall try to give – in chronological order – a survey over those papers and books, which are related to the study of extrapolation methods, beginning in the third century BC and ending with the famous paper of Richardson/Gaunt from 1927. Generally it has to be remarked that most of the authors did not take notice of each others work, which has led to an significant amount of re-discovering in the theory of extrapolation. In particular, this is true for the two groups of people working

on the computation of π on one side and on the numerical integration of differential equations and functions on the other, which developed over the centuries very similar numerical methods for the solution of their respective problem without knowing each other's work. To give a first example, Richardson's famous h^2 -extrapolation for the numerical solution of ODEs ([Richardson 1927]) is nothing else but the method for the computation of π , which was found by Huygens in [1654].

In some sense, the method sketched in Lemma 1 can be traced back until the work of Archimedes [250 BC]. Although Archimedes did not work on the field of extrapolation methods itself, his name must be quoted in this survey, since he founded a method for the approximative computation of π , which later on gave rise for the very important work of Huygens, Richardson/Gaunt, Kommerell and others.

Archimedes' method is well-described in many places (see e.g. Stiefel [1961], Engels [1979]), so we can be rather short here. The idea is to inscribe regular polygons in the unit circle and to take their areas (which Archimedes was able to compute) as an approximation to the area of the unit circle, hence for the number π . A remarkable connection to the modern Lemma 1 is the fact that he did increase the number of corners of the polygon not just somehow, but precisely *doubled* it in each step. Today, it is of course well-known that the area of the regular polygon with $2n$ corners on the unit circle is given by $A_{2n} = n \cdot \sin(\frac{\pi}{n})$ and possesses an AE of the type (1.1) with $h = 1/n, \rho_\nu = 2\nu, G = \pi$ and arbitrary m , see e.g. Walz [1987], [1992].

For many centuries this was the most widespread method for the computation of π , and the only advance that was made consisted in increasing the number n . For example, Ludolf van Ceulen (= from Cologne) in [1610] obtained 35 digits of π by computing the area of an polygon with 2^{62} vertices [Joyce 1971]!

The first methodical advance is due to Huygens [1654]; using geometrical arguments, he showed that the sequence $\{T_n\}$, defined by

$$T_n := (4 A_{2n} - A_n)/3 \quad (2.1)$$

converges faster to the limit π than the sequence $\{A_n\}$ itself does. So, Huygens found out the first step of the extrapolation procedure (1.2), since obviously (2.1) is nothing else but the step $k = 1$ of (1.2) in this special case.

The next milestone in the history of extrapolation methods is, without any doubt, the booklet of J.F.Saigey [1859], which seems unfortunately to have been overlooked for more than a century and was rediscovered by J.Dutka [1984]. Saigey developed, with

purely analytical methods, in particular without referring to Archimedes or Huygens, the existence of the AE for the sequence $\{A_n\}$, i.e. (with a slight change of notations)

$$A_n = \pi + \frac{c_1}{n^2} + \frac{c_2}{n^4} + \frac{c_3}{n^6} + \dots, \quad (2.2)$$

where the c_ν are fixed coefficients, and then derived from (2.2) his “higher approximations” to π , which turn out to be nothing else than the results of the extrapolation process (1.2): 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 (1.2) in *iterative form*; it must be noted that this was almost precisely 100 years before Rombergs paper [Romberg 1955] appeared.

In a historical note, Saigey remarked that he first had made a wrong conjecture concerning the denominators in his higher approximations: after having noted that the first ones equal 3 and 15, he had conjectured that the rule for constructing these denominators is

$$1 \cdot 3 = 3, \quad 1 \cdot 3 \cdot 5 = 15, \quad 1 \cdot 3 \cdot 5 \cdot 7 = 105, \dots$$

and so on, which is *wrong*. In a private communication, the engineer and geometer Guerin pointed out to him the correct rule, which is

$$4^1 - 1 = 3, \quad 4^2 - 1 = 15, \quad 4^3 - 1 = 63, \dots$$

Now we leave for a moment the problem of computing π and turn to the numerical integration of ordinary differential equations and real functions.

The first important work in this context is the famous “Deferred Approach to the Limit”, a paper which consists of two parts; the first one (“Single Lattice”) is due to L.F.Richardson [1927], the second one (“Interpenetrating Lattices”) to J.A.Gaunt

[1927]. Usually only the first part of the paper is quoted, and people therefore speak of *Richardson-extrapolation*. The method presented by Richardson and Gaunt is – also building on the work of Archimedes – a precise transcription of Huygens' method, which they obviously were not aware of, to the problem of integrating ordinary differential equations. They called it “ h^2 -extrapolation”, since they treated AEs of the form (1.1) with $\rho_\nu = 2\nu$ for all ν , and eliminated just the first ($= h^2$)-term of the expansion. It should be noticed that Richardson himself referred to a paper of Bugoljubov/Krylov [1926], in which the “deferred approach to the limit” can already be found (see Engels [1979]; since this paper is in Russian, it is widely unknown, and so far it was not possible for me to read it). Also, it is worth to be remarked that Richardson and Gaunt did not only use their method for the numerical solution of ordinary differential equations, but also for the general problem of accelerating the convergence of a sequence, and, for example, for the computation of Fourier coefficients (see also [Joyce 1971]). Just like Huygens before they did not try to bring their method into an iterative form, i.e. they did not want to eliminate further terms of the AE. Very interesting in this context is the remark of J.A.Gaunt, who writes that “... there would be no essential difficulty in extending the expansion beyond the fourth power of h ; but such a refinement would have little practical value” (!).

3. A Deeper Look into the Work of K. Kommerell

One of the most important publications in the context of extrapolation methods, which unfortunately seems to have been overlooked for all the years, is that of K.Kommerell [1936]. In spite of the fact that this book is referred to in the nice surveys by Engels [1979] as well as by Dutka [1984], we do think that still by far not all the deep ideas of Kommerell are exploited.

The great importance of his work lies in the fact that, building on the work of Huygens [1654], it already contains the *recursive algorithm* (1.2), applied to Archimedes' sequence $\{A_n\}$ as defined in the previous section (Kommerell [1936], p.37)! So, what Kommerell does is nothing else but to write down Romberg's method, here in the context of approximating π ! Therefore I am convinced that we should nowadays better speak of *Kommerell's method* when applying the extrapolation process (1.2).

And there is also another aspect which connects Kommerell's work with the one of Romberg, namely the fact that both define iteratively two approximating sequences, which *include* the limit value π resp. the exact value of the integral. We want to work out

now this so far unexploited part of Kommerell's work (for which he himself refers to the cardinal Cusanus). Please note that this approach is different from that of Archimedes resp. Huygens.

Starting with a regular polygon A_n (with n vertices) of fixed circumference U , one constructs the circle C which is circumscribed to A_n , and the regular polygon B_n which is circumscribed to C . Now one computes iteratively polygons with $2n$, $4n$, $8n, \dots$ vertices such that – in contrast to Archimedes' method – the circumference U remains fixed. This implies of course that the radii ρ_n of A_n and r_n of B_n converge to a circle with circumference U , i.e. we have

$$\lim_{n \rightarrow \infty} \rho_n = \lim_{n \rightarrow \infty} r_n = \frac{U}{2\pi}, \quad (3.1)$$

from which the number π can be computed. Kommerell did not give explicit formulae for ρ_n and r_n , but it is easy to see that, for all $n \geq 2$,

$$\begin{aligned} r_n &= \frac{U}{2n \sin(\pi/n)} \quad \text{and} \\ \rho_n &= r_n \cdot \cos(\pi/n). \end{aligned} \quad (3.2)$$

For practical use it is of great importance that the numbers r_n and ρ_n can be computed *recursively*. By geometrical considerations, Kommerell derived that, for all $n \geq 3$,

$$\begin{aligned} \rho_{2n} &= \frac{r_n + \rho_n}{2} \quad \text{and} \\ r_{2n} &= \sqrt{r_n \cdot \rho_{2n}}. \end{aligned} \quad (3.3)$$

Of course, the formulae (3.3) can also be obtained from (3.2). The sequences $\{\rho_n\}$ and $\{r_n\}$ are of particular interest, since we have the relations

$$\rho_2 < \rho_3 < \dots < \rho_n < \dots < \frac{U}{2\pi} < \dots < r_n < \dots < r_3 < r_2,$$

which imply that each pair (ρ_n, r_n) provides an inclusion of the true value.

But Kommerell was even not satisfied with this approximation, and he presented – as a new result – a convergence accelerating method; by subtil calculations he proved that the sequences $\{R_n\}$ and $\{S_n\}$, defined through

$$\begin{aligned} R_n &:= (4r_{2n} - r_n)/3 \quad \text{and} \\ S_n &:= (4\rho_{2n} - \rho_n)/3 \end{aligned} \quad (3.4)$$

provide better approximations to the limit value than the old ones. Now, the formulae (3.4) are again nothing else but the first step of the extrapolation process (1.2). From a

modern point of view, the application of (3.4) is justified by the fact that the values r_n and ρ_n possess an asymptotic expansion of the form (1.1) with $h = 1/n$, as can easily be deduced from (3.2). Kommerell himself illustrated the power of his method (3.4) by some numerical examples.

In addition, he proved that also the new sequences *include* the limit value, i.e. it is

$$R_n < \frac{U}{2\pi} < S_m$$

for all $n, m \in \mathbb{N}$. This is once more a deep connection with the later work of Romberg, who was also strongly interested in constructing such sequences, which include the true value. Unfortunately this aspect of both Kommerell's and Romberg's work also got lost in the meantime.

4. Developments since 1955. Final Remarks

The great breakthrough of extrapolation methods must of course be dated to the year 1955, when Romberg's fundamental and in the meantime famous paper on "Vereinfachte numerische Integration" (simplified numerical integration) appeared [Romberg 1955]. This paper has been reviewed in so many surveys that we do not want to do this here once more. It should only be remarked here that Romberg (who himself later on never wrote another paper on this topic) interestingly quotes the book of L. Collatz [1951] as the source of the iterative process (1.2) (for $\rho_k = 2k$).

As already pointed out, many authors denote (1.2) also as "generalized Romberg method" or just speak of "Romberg's principle". Although Romberg himself never thought of constructing a method for extrapolation or of giving a general principle for convergence acceleration (he "only" wanted to find new formulae for numerical integration), these names are justified at least inasmuch, as his paper inspired very many authors to work on this field and produce some nice results, which nowadays influence many parts of numerical analysis. Of course it is by far not possible to quote all successors of Romberg's paper, but we want to try at least to find the first and – to our opinion – most important ones of them.

In 1956, H. Bolton and H. Scoins published an extrapolation method in iterative form, here once again for the numerical solution of ODEs [Bolton/Scoins 1956]. The most important aspect of this paper is that they clearly worked out what is really needed for the applicability of the extrapolation, namely the existence of an asymptotic expansion!

Some years later, E. Stiefel wrote a paper on numerical quadrature methods, in which he put together and generalized in some sense the works of Archimedes, Kommerell and Romberg [Stiefel 1961].

Furthermore, we should mention the paper of H. Rutishauser [1963] on "Romberg's principle", where he very clearly points out that the extrapolation method (1.2) can be applied to *any* sequence of numbers $\{T(h)\}$, as long as this sequence possesses an asymptotic expansion. To illustrate this, he uses the method for the computation of $\log(x)$, for numerical differentiation and for the calculation of singular integrals.

In the following years, the number of papers which are concerned with extrapolation methods grew exponentially, and it is just impossible to give a detailed description of the further development; but we would like to mention the names of some outstanding researchers on this field, which are F. Bauer, C. Brezinski, R. Bulirsch, W. Gragg, T. Hävie, G. Mühlbach, H. Rutishauser, H. Stetter, E. Stiefel, J. Stoer, J. Wimp and P. Wynn. Those (and there are many of them, I suppose), which I have not quoted here, although I should have done so, I want to beg for their pardon.

Finally, it must be pointed out once more that the history of extrapolation methods was over the years characterized by a lot of disregard and re-discovering, what is quite a pity. Not only that many energy could have been saved, if the authors had taken notice of each others work, also some of the methods wear – from a historical point of view – the wrong names; for example, the Richardson-extrapolation process could have been denoted as *Huygens-extrapolation*, whereas Romberg's method maybe should have been named after *Kommerell* or *Saigey*. However, it must be said that Romberg's little paper gave the initialization for the rapid development of extrapolation methods in our times, and so this name is indeed justified.

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