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PREFACE

Preface

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This issue of *Numerical Algorithms* has a special flavor. It is not only devoted to applied mathematics as usual but also to the history of applied mathematics. Our Editor-in-Chief titled this issue "Extrapolation and Fixed Points." Here, "extrapolation" has to be understood as acceleration of the rate of convergence of sequences of scalars, vectors, matrices, or even tensors. This is intimately connected to root-finding techniques and fixed point methods for computing solution of nonlinear equations.

Acceleration of slowly converging sequences has been a concern for centuries, even long before the concept of limit was clearly and rigorously defined in the nineteenth century. A well-known example is the computation of π using series of which a multiple of π or of π^2 is the limit. This problem attracted a lot of interest starting in the seventeenth and eighteenth centuries and even earlier. For example, we have

$$\pi = 4 \sum_{k=0}^{\infty} (-1)^k \frac{1}{2k+1}.$$

The series on the right-hand side is very slowly convergent. If we sum the first 400 terms of this series, we obtain 3.139092657496014 in IEEE double precision floating point arithmetic, which is not a very good approximation of π. Using the ε-algorithm with the first 20 partial sums, we obtain 3.141592653589792 where only the last decimal digit is wrong, being 2 instead of 3.[1] This illustrates the usefulness of such acceleration methods. But, of course, there are better ways to compute π. We note in passing that Daniel Shanks, who is one of the researchers we are concerned with in

[1] This was computed with the `Epsfun` Matlab toolbox from Brezinski and Redivo-Zaglia

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this issue, was the first to compute π to 100,000 decimal places in a paper with John Wrench in 1961. It required 8 h 43 min on an IBM 7090 computer. In fact, all the decimals were printed in the paper published in 1962 in *Mathematics of Computation*. Nowadays, trillions of decimal places of π have been computed.

Even though we have now very fast computers, it is always of interest to study methods for accelerating the convergence of sequences. Moreover, these methods have connections with other very interesting mathematical topics like continued fractions and Padé approximants. As often, to understand today's research, it is useful to look at the past. This is what is done in this issue concerning extrapolation and acceleration.

This issue is dedicated to the fond memory of Peter Wynn (1931–2017) who was the father of the famous ε-algorithm. Claude Brezinski who used to know Wynn quite well in the 1970s and 1980s is sharing with us some remembrances of his relationship with Wynn.

The second paper by C. Brezinski and M. Redivo-Zaglia is about the mathematics and the history of Aitken's Δ^2 process, Shanks' transformation, Wynn's ε-algorithm, and related fixed point methods. They first give a review of the mathematical theory of these methods and their relations to other topics, for instance, Padé approximants. Then, they give details about how these methods were derived as well as an analysis of the papers of the main contributors. These methods are often used to accelerate the convergence of fixed points iterations like the basic Picard iteration for solving nonlinear problems. The authors discuss Steffensen's method and its generalizations as well as the works of Samuelson, Anderson, and Pulay. They also consider the successors of these early contributors and the extensions of the acceleration methods to vectors and sequences in vector spaces. They describe the topological ε-algorithm (TEA) and its recent simplification STEA, as well as the vector ε-algorithm (VEA), the minimal polynomial extrapolation algorithm (MPE), the modified minimal polynomial extrapolation algorithm (MMPE) and the reduced rank extrapolation algorithm (RRE). Finally, they provide biographical information about Aitken, Anderson, Cabay, Eddy, Jackson, Kaniel, Lemaître, Maxwell, O'Beirne, Padé, de Prony, Pulay, Samuelson, Shanks, Steffensen, and Wynn as well as an extensive list of references. Historical details on the development of the methods directly provided by some of the main contributors are also given.

In 1965, D.G. Anderson proposed an algorithm for solving fixed point problems. Anderson was interested in problems arising from solving nonlinear integral equations and his goal was to develop an algorithm which converges faster than the basic Picard iteration. He called the proposed method the Extrapolation Algorithm. Later on, this algorithm has been called Anderson Acceleration (AA) in the applied mathematics community and Anderson Mixing in the computational quantum chemistry community. Even though it can be considered as an acceleration method, AA is different from other methods which compute iterates of the basic iteration method and then combine them in some sense to obtain faster convergence. On the contrary, AA produces its own sequence of approximations of the solution. In his essay in this issue, D.G. Anderson describes his method in great details, particularly how the solution of the least squares problem to be solved is obtained using Householder reflections, with pivoting and adaptive regularization. Then, he analyzes and discusses the results of some of the papers that have been written subsequently about AA. Fortunately, this essay gives us a first-hand account about a well-known and interesting algorithm by its author himself.

In his paper, Hervé Le Ferrand explains how Georges Lemaître rediscovered independently Aitken's Δ^2 process. He used a different starting point than Aitken for the development of his rational iteration method. Lemaître was a quite interesting man. He was a physicist, an astronomer and cosmologist, a mathematician, and a catholic priest. He is most well-known for being one of the pioneers of the big bang and the expansion of the universe theory. He called his theory the hypothesis of the primeval atom. This point of view seems quite unusual for a catholic priest. In fact, this led him to have some troubles and disputes with Pope Pius XII but Lemaître was against mixing science with religion. He also had a strong interest in the development of computers and numerical methods as you will see in Le Ferrand's paper.

The paper by A. Messaoudi, M. Errachid, K. Jbilou, and H. Sadok is not about history but concerned with a topic closely related to extrapolation, that is, interpolation. A new algorithm is proposed for the general Hermite interpolation problem. Given distinct points x_j on the real line and corresponding to each point given real values $y_{j,k}$, we would like to compute the coefficients of a polynomial such that its values and the values of its derivatives at x_j are equal to the values $y_{j,k}$. Moreover, the number of the given values may be different for every point x_j.

The classical algorithm for solving this problem uses generalized Lagrange interpolation polynomials. The formulation of the problem proposed in this paper uses different tools: Schur complements, determinants, and the Sylvester identity. The interpolation polynomial can be expressed as a Schur complement and the Sylvester identity is used to compute it recursively. This yields recurrence relations for the polynomial and a first algorithm involving auxiliary polynomials that can also be computed recursively. Considering the properties of these auxiliary polynomials, the algorithm can be further simplified. An advantage of the new method is that it does not require additional storage besides what is used for the problem data. Moreover, adding or removing a point (which is known as updating or downdating the solution) can be done easily without having to recompute everything from scratch.