Contemporary Mathematicians

Claude Brezinski
Ahmed Sameh
Editors

Walter Gautschi

Selected Works with Commentaries

Volume 3

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Contemporary Mathematicians

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Walter Gautschi, Volume 3

Selected Works with Commentaries

Birkhäuser

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Walter Gautschi, 2009
hiking in the Swiss alps

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26.3 [35] An Application of Minimal Solutions of Three-Term Recurrences to Coulomb Wave Functions, *Aequationes Math.* 2, 171–176 (1969) 91
26.4 [37] (with B. J. Klein) Recursive Computation of Certain Derivatives — A Study of Error Propagation, *Comm. ACM* 13, 7–9 (1970) 98
26.5 [135] Is the Recurrence Relation for Orthogonal Polynomials Always Stable?, *BIT* 33, 277–284 (1993) 102
26.6 [150] The Computation of Special Functions by Linear Difference Equations, in *Advances in difference equations* (S. Elaydi, I. Győri, and G. Ladas, eds.), 213–243 (1997) 111

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27.2 [54] Global Error Estimates in "One-Step" Methods for Ordinary Differential Equations, *Rend. Mat.* (2) 8, 601–617 (1975) (translated from Italian) 162
27.3 [73] (with M. Montrone) Multistep Methods With Minimum Global Error Coefficient, *Calcolo* 17, 67–75 (1980) (translated from Italian) 178

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28.1 [141] Algorithm 726: ORTHPOL — A Package of Routines for Generating Orthogonal Polynomials and Gauss-type Quadrature Rules, *ACM Trans. Math. Software* 20, 21–62 (1994); Remark on Algorithm 726, *ibid.* 24, 355 (1998) 188
28.2 [179] Orthogonal Polynomials, Quadrature, and Approximation: Computational Methods and Software (in Matlab), in *Orthogonal polynomials and special functions — computation and applications* (F. Marcellán and W. Van Assche, eds.), 1–77, Lecture Notes Math. 1883 (2006) 231

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29.1 [74] A Survey of Gauss–Christoffel Quadrature Formulae, in *E. B. Christoffel — the influence of his work in mathematics and the physical sciences* (P. L. Butzer and F. Fehér, eds.), 72–147 (1981) 311

29.2 [91] (with J. Wimp) In Memoriam: Yudell L. Luke June 26, 1918 – May 6, 1983, *Math. Comp.* 43, 349–352 (1984).................................... 388
29.3 [101] Reminiscences of My Involvement in de Branges's Proof of the Bieberbach Conjecture, in *The Bieberbach conjecture* (A. Baernstein II, D. Drasin, P. Duren, and A. Marden, eds.), 205–211, Proc. Symp. on the Occasion of the Proof, Math. Surveys Monographs 21, American Mathematical Society (1986).. 393
29.4 [143] The Work of Philip Rabinowitz on Numerical Integration, *Numer. Algorithms* 9, 199–222 (1995).. 401
29.5 [144] Luigi Gatteschi's Work on Special Functions and Numerical Analysis, in *Special functions* (G. Allasia, ed.), *Annals Numer. Math.* 2, 3–19 (1995) 426
29.6 [170] The Interplay Between Classical Analysis and (Numerical) Linear Algebra — A Tribute to Gene H. Golub, *Electron. Trans. Numer. Anal.* 13, 119–147 (2002) 444
29.7 [183] Leonhard Eulers Umgang mit langsam konvergenten Reihen, *Elem. Math.* 62, 174–183 (2007)... 474
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29.9 [186] On Euler's Attempt to Compute Logarithms by Interpolation: A Commentary to His Letter of February 16, 1734 to Daniel Bernoulli, *J. Comput. Appl. Math.* 219, 408–415 (2008) 500
29.10 [187] Leonhard Euler: His Life, the Man, and His Works, *SIAM Rev.* 50, 3–33 (2008). [Also published in *ICIAM 07, 6th International Congress on Industrial and Applied Mathematics, Zürich, Switzerland, 16–20 July 2007* (R. Jeltsch and G. Wanner, eds.), 447–483, European Mathematical Society, (2009). Chinese translation in *Mathematical Advance in Translation* (2–3) (2008).].. 509
29.11 [189] (with C. Giordano) Luigi Gatteschi's Work on Asymptotics of Special Functions and Their Zeros, in *A collection of essays in memory of Luigi Gatteschi* (G. Allasia, C. Brezinski, and M. Redivo-Zaglia, eds.), *Numer. Algorithms* 49, 11–31 (2008) 541
29.12 [196] Alexander M. Ostrowski (1893–1986): His Life, Work, and Students, in *math.ch/100 Swiss Mathematical Society 1910–2010* (B. Colbois, C. Riedtmann, and V. Schroeder, eds.), 257–278, European Mathematical Society, (2010) 563
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30.2 [96] (with B. N. Flury) An Algorithm for Simultaneous Orthogonal Transformation of Several Positive Definite Symmetric Matrices to Nearly Diagonal Form, *SIAM J. Sci. Statist. Comput.* 7, 169–184 (1986) 617
30.3 [124] A Class of Slowly Convergent Series and Their Summation by Gaussian Quadrature, *Math. Comp.* 57, 309–324 (1991) 634
30.4 [125] On Certain Slowly Convergent Series Occurring in Plate Contact Problems, *Math. Comp.* 57, 325–338 (1991) 651
30.5 [149] (with J. Waldvogel) Contour Plots of Analytic Functions, Ch. 25 in *Solving problems in scientific computing using Maple and Matlab* (W. Gander and J. Hřebíček, eds.), 3d ed., 359–372, Springer, Berlin, 1997. [Chinese translation by China Higher Education Press and Springer, 1999; Portuguese translation of 3d ed. by Editora Edgard Blücher Ltda., São Paulo, 2001; Russian translation of 4th ed. by Vassamedia, Minsk, Belarus, 2005.] 666
30.6 [175] The Hardy–Littlewood Function: An Exercise in Slowly Convergent Series, *J. Comput. Appl. Math.* 179, 249–254 (2005) 681
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Part I

Commentaries

In all commentaries, reference numbers preceded by “GA” refer to the numbers in the list of Gautschi’s publications; see Section 4, Vol. 1. Numbers in boldface type indicate that the respective papers are included in these selected works.

21

Linear recurrence relations

Lisa Lorentzen

Walter Gautschi is a giant in the field of linear recurrence relations. His concern is with stability in computing solutions $\{y_n\}_{n=0}^{\infty}$ of such equations. Suppose the recurrence relation is of the form

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0 \qquad \text{for} \quad n = 1, 2, 3, \ldots. \tag{21.1}$$

It seems so deceivingly natural to start with values or expressions for y_0 and y_1, and then compute y_2, $y_3, \ldots$ successively from (21.1). However, this does not always work. Yet, in every new generation of mathematicians or users of mathematics, along come some incorrigible optimists with a naive trust in this method. We are happy, of course, for every new optimist in the field; mathematicians do not get far without optimism, stamina, creativity, and enthusiasm. But the new ones can definitely benefit from some sensible guidance. And what they should do, is to start with Walter Gautschi's *SIAM Review* paper [GA**29**] on three-term recurrence relations from 1967. This is what most people do, and this is what I did when I started my study of continued fractions. Continued fractions and recurrence relations indeed share a substantial intersection which, however, calls for some degree of alertness.

So what can go wrong if one computes a solution as described above? Several things, says the Master. But the worst scenario occurs if one tries to compute a solution $\{f_n\}_{n=0}^{\infty}$ of (21.1) which happens to be *minimal*. A sequence $\{f_n\}$ is a minimal solution if (21.1) has a second solution $\{y_n\}$ for which $f_n/y_n \to 0$. This second solution is then called a *dominant* solution. The solution space of (21.1) is obviously a two-dimensional vector space, so a small error in the initial data, for example a rounding error, changes $\{f_n\}$ to some dominant solution $\{\alpha f_n + \beta y_n\}$, $\beta \neq 0$, with totally different asymptotic behavior. The discrepancy between f_n and $\alpha f_n + \beta y_n$ may be catastrophic after only a few computational steps, as so convincingly demonstrated by Gautschi.

Not every such recurrence relation has a minimal solution, and one may think that the subspace of minimal solutions is so small – if it exists at all – that the chance

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of encountering one is also minimal. But that is not at all the case. On the contrary, as so often in mathematics, special cases are often the most interesting ones. A number of important sequences of special functions are indeed minimal solutions of linear recurrence relations. And here we are at the heart of the problem: how can we compute minimal solutions stably and efficiently?

For recurrence relations of the form (21.1) the answer can be found in continued fraction theory: the continued fraction

$$\frac{-b_1}{-a_1-}\,\frac{b_2}{-a_2-}\,\frac{b_3}{-a_3-}\cdots = \frac{b_1}{a_1-}\,\frac{b_2}{a_2-}\,\frac{b_3}{a_3-}\cdots \tag{21.2}$$

has approximants

$$\frac{b_1}{a_1-}\,\frac{b_2}{a_2-}\cdots\frac{b_n}{a_n} = \frac{A_n}{B_n},$$

where $\{A_{n-1}\}_{n=0}^{\infty}$ and $\{B_{n-1}\}_{n=0}^{\infty}$ are solutions of (21.1) with initial conditions

$$A_{-1}=1,\; A_0=0; \quad B_{-1}=0,\; B_0=1.$$

Gautschi observes the following connection between the continued fraction (21.2) and minimal solutions of (21.1), and attributes it to Pincherle, who proved it in an obscure 1894 paper written in Italian: there exists a minimal solution $\{f_n\}$ of (21.1) satisfying $f_0 \neq 0$ if and only if the continued fraction (21.2) converges to a finite limit. In that case, moreover,

$$r_n := \frac{f_n}{f_{n-1}} = \frac{-b_n}{a_n-}\,\frac{b_{n+1}}{a_{n+1}-}\cdots, \quad n=1,2,3,\ldots, \tag{21.3}$$

provided $f_n \neq 0$ for all n.

This immediately suggests a stable way to compute minimal solutions, namely to compute the continued fractions $r_n, r_{n-1}, \ldots, r_1$ in (21.3) and then f_n from

$$f_n = r_n r_{n-1}\cdots r_1 f_0,$$

assuming f_0 is known. For more details, see also Section 11.1, Vol. 2.

But things are not always as easy as they may look on paper. It took a Walter Gautschi to sort out the problems and work this simple idea into useful, reliable algorithms. As always, it is the stability analysis, controlling the error, that takes ingenuity. Via some very nice twists and tricks — see, e.g., Gautschi's treatment in [GA**29**, Sec. 7] and [GA**35**] of the three-term recurrence relation satisfied by Jacobi polynomials of purely imaginary parameters and argument — his algorithms work like a dream; these are not just algorithms on paper.

But what if f_0 is unknown? Also this problem was handled by Gautschi: he replaced the condition "f_0 known" by "$\sum_{n=0}^{\infty}\lambda_n y_n$ known", with known coefficients λ_n – a situation one often meets in the theory of special functions. Also this was incorporated into his algorithms. Of course, Walter Gautschi has also treated linear recurrence relations of other forms (for example, see [GA**150**]) with the same care, and he has applied them to compute important sequences of special functions, orthogonal polynomials and interesting integrals. What is so very nice about his algorithms is that they come with such a very careful and convincing stability analysis. He has forever changed the way one looks at recurrence relations and continued fractions.

People do not only read his books and papers – they really use his results. His contributions to the *Handbook of Mathematical Functions* by Abramowitz and Stegun are frequently consulted, both his Chapter 7 on the error functions and Fresnel integrals and Chapter 5 which he wrote with W.F. Cahill on the exponential integral and related functions. Not to mention his algorithms for the complex error function, the incomplete gamma functions, the Fresnel integrals etc. in the NAG-library and other places (cf. Section 6.1, Vol. 1). To me, the very fact that so many people talk with ease about minimal solutions and stability analysis as if they had known about it all their lives, is particularly gratifying. And this happens not only in conferences on recurrence relations, but on special functions, orthogonal polynomials, continued fractions, and applied mathematics, to mention just a few.

You know your ideas have made a deep impression when fellow mathematicians begin to name concepts after you. And in the literature one finds references to the "Gautschi algorithm" number so and so, the "Gautschi method" for stability analysis, and even (more amusingly) the "Gautschi-type method" as if there were some people out there of "Gautschi-type". I think one would have a hard time finding anyone like Walter Gautschi. After the very sad death of his twin brother, Walter is unique. His clear mind and his creativity penetrate all his work, and also his oral as well as written presentations. So I end this short exposition with a serious advice: dig in and enjoy.

22

Ordinary differential equations

John Butcher

These days everyone talks about "impact" as something that can be measured in terms of citations within a year or two, but the impact of many important contributions to science can be looked at in other, more perceptive, ways. I believe this is especially true of [GA**14**]. This paper is forward-looking to the extent that its importance has become recognised more and more as time has passed. In my opinion the impact of this contribution has been tremendous. Over the years it has become known as a pioneering paper in the fitted type of approach to the solution of initial value problems. It has been referenced directly soon after its publication but even more so in recent years. It is related to exponential integration, to exponential fitting, and to modern approaches to the solution of highly-oscillatory problems. The ideas and results in the original paper have been rediscovered independently by later authors, but the depth and scholarship in Gautschi's exposition are unmatched. Here are the key definitions near the start of the paper.

A linear functional L in $C^s[a,b]$ is said to be of *algebraic order* p if

$$Lt^r = 0 \qquad (r = 0, 1, \ldots, p);$$

it is said to have *trigonometric order* p*, relative to period* T, if

$$L1 = L\cos\left(r\tfrac{2\pi}{T}t\right) = L\sin\left(r\tfrac{2\pi}{T}t\right) = 0 \qquad (r = 1, 2, \ldots, p).$$

On this foundation, the paper goes on to analytical questions concerned with the existence of trigonometric methods, the actual construction of methods, especially of Adams and Störmer types, numerical investigations, and the sensitivity of numerical results to the value of T in relation to the exact period.

The chapter [GA15] from S*urvey of numerical analysis*, McGraw-Hill, New York (1962), written in collaboration with H. A. Antosiewicz, surveys the state of knowledge, at the time, of numerical methods for ordinary differential equations. This work set the standard for theoretical expositions on this subject, appearing as it did, a short time prior to the monograph of P. Henrici. Although the work of

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Curtiss and Hirschfelder had appeared several years earlier, it was not yet known and appreciated in the mathematical community. However, a cautionary example problem,

$$\frac{dy}{dx} = \begin{pmatrix} 0 & 1 \\ 10a^2 & 9a \end{pmatrix} y, \qquad y(0) = \begin{pmatrix} 1 \\ -a \end{pmatrix},$$

is presented which, for $a > 0$, leads to approximations to the solution $\exp(-ax)y(0)$ being eventually, but inevitably, overshadowed by terms which grow like $\exp(10ax)$. After stiffness had become a recognised phenomenon, it would have become more illuminating to consider $a < 0$; in this case the difficulty would not have been that the required solution is buried amongst dominant alternative solutions, but that the required solution has now become dominant even though its dominance is lost in computations with classical explicit methods.

Looking now at [GA**54**], we are reminded of a crucial time in the history of Runge–Kutta methods. This review paper acknowledged recent work, by Fehlberg and others, in constructing embedded methods for the purpose of step-size control. It appeared at a time when Henrici's monograph was becoming recognised as a model for exposition in numerical analysis and took the rigorous mathematical style a step further. But global error bounds based on very reasonable assumptions, such as the Lipschitz condition, do not necessarily give tight error bounds. This beautiful paper viewed retrospectively, encapsulates all these ideas.

Paper [GA56] contains short and elegant proofs of the asymptotic behaviour of the coefficients in Adams and other integration formulae.

For a linear k-step method (ρ, σ), where ρ is given, with zeros satisfying $1 = \zeta_1 \geq |\zeta_2| \geq |\zeta_3| \geq \cdots \geq |\zeta_k|$, there is a unique choice of σ to give order $p = k+1$. The aim of the paper [GA**73**] is to determine the method for which $|\zeta_i| \leq \gamma$, $i = 2, 3, \ldots, k$, $0 \leq \gamma < 1$, that has minimal global error constant. It is shown that in the optimal solution, $\zeta_i = -\gamma$, $i = 2, 3, \ldots, k$. Ramifications of the result are studied in detail.

Somewhere between the appearance of the first and last paper surveyed here, I met Walter Gautschi in person. I was once his guest at Purdue and met him from time to time at conferences. I have come to know him as a kind and courteous person as well as a scholarly, knowledgeable, and original mathematician.

23

Computer algorithms and software packages

Gradimir V. Milovanović

During the preparation of the *Handbook of Mathematical Functions*, under the direction of Milton Abramowitz at the Bureau of Standards (now the "National Institute of Standards and Technology"), Walter Gautschi, then a young research mathematician, joined this project in 1956. This was the starting point of a period of intense work with special functions. During the 1960s, in addition to theoretical work in several domains of special functions (see Section 6, Vol. 1), Walter developed a number of computer algorithms evaluating special functions: the gamma function and incomplete beta function ratios [GA22], Bessel functions of the first kind [GA23], Legendre functions [GA24], derivatives of e^x/x, $\cos(x)/x$, and $\sin(x)/x$ [GA27], [GA38], regular Coulomb wave functions [GA28], [GA33], the complex error function [GA36], repeated integrals of the coerror function [GA60], and incomplete gamma functions [GA69].

In 1968 Gautschi began to write computer algorithms for Gaussian quadrature formulas, the first being the one in [GA32]. This opened the door for extensive work on orthogonal polynomials and their applications (see Sections 11, 12, 14, 15 in Vol. 2), but also for developing related software. The first major software package, `ORTHPOL`, appeared in 1994 as Algorithm 726 in [GA**141**]. It contains routines, written in FORTRAN, that produce the coefficients in the three-term recurrence relation for arbitrary orthogonal polynomials as well as nodes and weights of Gauss-type quadrature rules. A more specialized package, `GQRAT` [GA159], produced Gauss quadrature rules which are exact for a combination of polynomials and rational functions. They are useful for integrating functions that have poles outside the interval of integration.

The package `ORTHPOL`, as well as the subsequent package `OPQ` of MATLAB routines, both made available on the internet (`http://www.cs.purdue.edu/archives/2002/wxg/codes`), led to a significant boost in the computational use and application of orthogonal polynomials. The companion package `SOPQ`, also available on the internet, contains symbolic versions of some of the more important routines in `OPQ`. They can be used for high-precision work in orthogonal polynomials and Gaussian

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quadrature. A similar package in MATHEMATICA is `OrthogonalPolynomials` [1] (see also [2]).

A very comprehensive account of computational methods and software in MATLAB is provided in [GA**179**]. It illustrates the use of the `OPQ` routines in an elegant, interesting, and methodical way.

References

[1] Aleksandar S. Cvetković and Gradimir V. Milovanović. The Mathematica package "OrthogonalPolynomials". *Facta Univ. Ser. Math. Inform.*, 19:17–36, 2004.

[2] Gradimir V. Milovanović and Aleksandar S. Cvetković. Special classes of orthogonal polynomials and corresponding quadratures of Gaussian type. *Math. Balkanica*, 26(1–2):169–184, 2012.

24

History and biography

Gerhard Wanner

24.1. Euler

The ICIAM Congress 2007, held in Zürich, happened to be in the year of Euler's 300th anniversary. It was then clear to the organizers, that one of the invited talks should be dedicated to Euler and Euler's work. Fortunately, Walter Gautschi accepted this invitation and presented a fascinating talk on Euler's life, his personality, an overview of his work and some selected topics in more detail. This took place in the largest lecture hall (the "Turnhalle"), filled up to the last seat. I still remember the total silence in the audience, when Gautschi ran a video of an Euler gear transmission, turning, as he said, "without any noise". An expanded version of this talk [GA**187**] was prepared for the proceedings of the congress and, by mutual agreement between the publishers, also appeared in *SIAM Review* 2008, followed by a Chinese translation. Two particular items from this talk, Euler's treatment of slowly converging series and Euler's discovery of the convergence to a wrong limit of interpolatory polynomials for the logarithm, a phenomenon which 100 years later became known as q-theory, led to two separate publications, [GA**183**] and [GA**186**].

24.2. The Bieberbach conjecture

An extraordinary story is told in [GA**101**], where Gautschi, who had worked all his life on numerical analysis, quadrature, and orthogonal polynomials, suddenly had the occasion to complete, in a couple of days, Louis de Branges's proof of a long-standing conjecture in pure mathematics. This conjecture, an inequality for the Taylor coefficients of a 1-1 holomorphic mapping from a circle to a simply connected domain, was formulated by Bieberbach in 1916 during his early work on the Riemann mapping theorem. During many decades, this conjecture had resisted the efforts of the foremost experts in complex analysis. Louis de Branges finally managed to reduce this conjecture to inequalities for integrals of Jacobi polynomials and thought that Walter Gautschi, with his algorithms and computers, could help to

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verify them. Gautschi not only did a lot of computer computations, but eventually found out that the inequalities had been proved a decade earlier by R. Askey and G. Gasper. I remember that P. Henrici, who lectured on this proof in January of 1985 in Stockholm on the occasion of Dahlquist's 60th anniversary, concluded his talk with the observation that a mathematician cannot know everything, but that "it is always important to know where to ask".

24.3. Survey articles

Walter Gautschi, with his broad knowledge of numerical analysis and his many personal contacts with leading experts, was (and is) in excellent position to write extraordinarily clear survey articles. Even when he wrote on a particular scientist, his narrative always turned into a beautiful and clear exposition of the underlying mathematics. We therefore collect them together: the article [GA**74**] on Gauss-Christoffel quadrature, the article [GA**143**] on Philip Rabinowitz and numerical integration, the papers [GA**144**] on 2d-iterations and numerical quadrature and [GA**189**] on asymptotics and estimation of zeros of special functions summarizing work of Luigi Gatteschi, and finally [GA**170**], the interplay between classical analysis and numerical linear algebra as a special tribute to Gene H. Golub. The same subject is dealt with in Gautschi's commentary [GA**184**], written for the edition of the selected works of Gene H. Golub.

Finally, in [GA**201**], Gautschi tells the story of how he came into scientific contact with G. V. Milovanović (we all have experienced, as referees, receiving a paper which immediately could be simplified and improved; authors then often react angrily, but in other situations such as the one described here, this was the starting point of a long friendship and collaboration). Gautschi's paper then continues with a description of Milovanović's work on Gaussian integration with unusual weight functions, and moment-preserving spline approximation.

24.4. Biography

The biography, which Gautschi wrote, was for his esteemed teacher Alexander M. Ostrowski [GA**196**], one of the great mathematicians of the 20th century. This paper is an extended version of an earlier paper [GA171] (not reproduced in these volumes) written in Italian. This account of Ostrowski's life and work, carefully written by one of his last students, is highly interesting and needs no further comment.

25

Miscellanea

Martin J. Gander

Here, five "miscellaneous" papers of Walter Gautschi are commented on, [GA**96**, GA**124**, GA**125**, GA**175**, GA**197**], preceded by some personal reminiscences.

I encountered Walter Gautschi's work several years before I encountered him in person. I was a PhD student at Stanford and taking a course given by Gene Golub on orthogonal polynomials and quadrature. Several faculty members were also taking this course, among them Andrew Stuart, who became my PhD supervisor, and Alan Karp. During the lectures, Alan Karp posed an interesting problem of computing Gauss quadrature nodes and weights for difficult weight functions arising in radiative transfer. I immediately put to work what I had learned in class, and failed, since all the methods we had seen were becoming rapidly unstable, and it was not possible to compute the recurrence coefficients of the required orthogonal polynomials to sufficiently high accuracy. So I started to search the literature and came across a paper of Walter Gautschi, [GA**141**], which describes precisely the problems I was working on, and also proposes an ingenious discretization procedure, which allowed me to replace the unstable approaches I tried before by orthogonal transformations, which are naturally numerically stable. This procedure allowed us to compute very effectively high-order Gauss quadrature rules for all important weight functions in this application, and led to the short paper [3].

I met Walter Gautschi for the first time on Sunday, April 26, 1998, when he came for a seminar to the École Polytechnique in Paris, where I was doing my postdoc. We hit it off immediately, and when our twins were born in Montreal, this added a further common bond, since Walter Gautschi also had a twin brother, Werner Gautschi, a very talented mathematician as well, who unfortunately passed away too early in life. When I moved to Geneva for a full professorship, I invited Walter Gautschi to give a talk at our mathematics colloquium, and, happily, he agreed to come. He gave a very well-received talk about "The spiral of Theodorus, numerical analysis, and special functions". To my delight, I found this talk again in

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one of the papers I was assigned to study more closely in this tremendous enterprise of commenting on the selected works of Walter Gautschi. I will do this, however, in chronological order, so the Theodorus paper will come last.

25.1. The FG algorithm

This paper, [GA**96**], which is joint work with Bernard Flury from the University of Bern, appeared when I was still in high school! It is very atypical for the work of Walter Gautschi I am familiar with, dealing with a topic from numerical linear algebra. For a given set of symmetric positive definite matrices $A_1, A_2, \ldots, A_k$, the authors present an iterative algorithm to compute an orthogonal transformation B such that the matrices $B^T A_1 B, B^T A_2 B, \ldots, B^T A_k B$ are as close to diagonal as possible. In order to measure this "closeness", they introduce (and motivate) the function

$$\Phi(A_1, A_2, \ldots, A_k; n_1, \ldots, n_k) := \prod_{i=1}^{k} [\det(\mathrm{diag} A_i)]^{n_i} / [\det(A_i)]^{n_i},$$

where the n_i are given numbers. The best choice of B is one for which

$$\Phi(B^T A_1 B, B^T A_2 B, \ldots, B^T A_k T; n_1, \ldots, n_k) \longrightarrow \min .$$

In order to compute an approximate minimizer, the authors introduce the FG(Flury–Gautschi) algorithm, which consists of an outer iteration F and an inner iteration G. The algorithm is described in pseudocode, and the authors prove convergence of the algorithm. In the case $k = 1$, their algorithm reduces to the Jacobi method. In addition to the convergence of the two procedures, the authors also analyze under which conditions the solution is unique, and they give several hints for improving the algorithm.

Unfortunately, there was no implementation of the algorithm given in the paper[1]. Because of my interest in the algorithm, and since several details of the implementations were only addressed by comments, I decided to implement the algorithm myself in Matlab (see `http:/www.unige.ch/~gander/FG.php`)[2]. The algorithm was tested on the same example as given in the paper. It took quite a while to obtain the same results, because the implementation of the stopping criterion, based, as it was, on a comparison of eigenvectors becoming close, is tricky since normalized eigenvectors are only unique up to a sign and also come numerically in an arbitrary order. The current implementation now faithfully reproduces the authors' Fortran results. Their implementation on a CDC 170/855, in 1986, took 0.07 seconds of CPU time for this example to be executed. In Matlab on my Thinkpad T60, in

[1] With the help of Walter, we later found the Fortran implementation in [2].

[2] Many thanks to Hui Zhang, who also implemented the algorithm independently, so we could compare.

2012, the same example takes 0.03 seconds of CPU time. One wonders where all the computing power has gone these days[3].

Another test, which illustrates why the identity matrix as an initial guess of B can fail in the F-algorithm, is to simultaneously diagonalize a stiffness and a mass matrix (where this is actually possible)[4]. Specifically, the matrices

$$A_1 = \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 4 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 4 \end{bmatrix}$$

give rise to an infinite loop when the initial guess of B in the F-algorithm is the identity matrix, and one needs to use an alternative random initial guess.

I could imagine that such an algorithm would find many users if it were generally available in Matlab, since the simultaneous diagonalization of matrices is an important task.

25.2. Slowly convergent series

The relevant paper on this topic, [GA**124**], as well as the paper [GA**125**] in the next subsection, are more in the core area —numerical quadrature — of Walter Gautschi's research interests. The problem is to sum the series

$$S_0 = \sum_{k=1}^{\infty} k^{\nu-1} r(k), \quad S_1 = \sum_{k=1}^{\infty} (-1)^{k-1} k^{\nu-1} r(k),$$

where $r(k)$ is a rational function. By using a preliminary partial fraction decomposition, Walter shows that it suffices to consider r of the form

$$r(s) = \frac{1}{(s+a)^m}, \qquad \Re a \geq 0, \quad m \geq 1.$$

Such series can be transformed into integrals by writing the fraction as a Laplace transform and then changing the order of summation and integration. The result is a weighted integral of an entire function; it then remains to determine Gauss quadrature rules for the respective weight function. With the hand of the master, Walter determines the three-term recurrence coefficients for the required orthogonal polynomials, which, as I experienced myself, are not always easy to compute to high precision. From these, one can easily obtain the required Gauss quadrature rules. He then illustrates the resulting fast summation procedure in the case of five infinite series, of which the first was communicated to Walter by Professor P. J. Davis who came upon it in his study of spirals, a topic we will again encounter in the fifth paper.

[3] Compilation would make this certainly much faster.

[4] Many thanks to Ivan Graham for suggesting this useful example during a conference in Urümqi in August 2012.

25.3. Slowly convergent series occurring in plate contact problems

This paper is a continuation of the previous paper, and it appeared in the same journal, right after the previous one. The subject is again the fast summation of infinite series, this time of the form

$$\sum_{k=0}^{\infty}(2k+1)^{-p}z^{2k+1},$$

where z is complex with $|z| \leq 1$ and $p = 2, 3$, and also of the more difficult forms

$$\sum_{k=0}^{\infty}(2k+1)^{-p}\,\frac{\cosh((2k+1)x)}{\cosh((2k+1)b)}\,, \quad \sum_{k=0}^{\infty}(2k+1)^{-p}\,\frac{\sinh((2k+1)x)}{\sinh((2k+1)b)}\,,$$

where $0 \leq x \leq b$. Such series occur in the mathematical treatment of unilateral plate contact problems. After treating some special cases, Walter again uses the device of introducing a Laplace transform, but now only for part of the general term of the series. Interchanging summation and integration, as in the earlier paper, leads to a weighted integral with a weight function similar to the one in the previous paper. There are, however, cases for the parameters where Gauss quadrature is no longer effective, and Walter shows how a further transformation leads to an integral which can be effectively evaluated using a backward recursion scheme. Faithful to his working style, he gives the needed recurrence coefficients to high accuracy, and then shows two fully worked out examples to illustrate the technique.

25.4. The Hardy–Littlewood function

In the short 6-page note [GA**175**], Walter Gautschi gives a summary of his conference presentation at the birthday conference for Olav Njåstad. The topic was the summation of the series

$$H(x) = \sum_{k=1}^{\infty}\sin(x/k)/k, \tag{25.1}$$

which is important in the study of the polygamma functions. Walter first shows how the summation can be performed using orthogonal polynomials and polynomial/rational Gauss quadrature (cf. Section 15.4, Vol. 2), again applying the Laplace transform device. In a first approach, he obtains a formulation in terms of modified Bessel functions of order zero, the power series expansion of which, however, is only suitable for relatively small positive values of x, because otherwise severe cancellation errors make the approach numerically useless. As an alternative, Walter rewrites the expression obtained by using an integral representation of the Bessel function, in which case the trapezoidal rule can be used effectively and without cancellation. He then also uses rational Gauss–Laguerre quadrature directly in the original formulation, and with this approach the range of x-values can be substantially enlarged before cancellation problems set in. Walter finally shows a completely different approach, based on direct summation of the first $n \approx x$ terms combined with an acceleration procedure, which is very effective for large values of x.

As it turned out, this short paper became the major inspiration for a recent publication by Kuznetsov [5] on asymptotic approximations to the Hardy–Littlewood function. Kuznetsov's goal was to find a value of x for which $H(x)$ in (25.1) satisfies $H(x) < -\pi/2$, in order to provide an explicit counterexample to a conjecture of Clark and Ismail. (The value of x found was extremely large, of the order 10^{21}!) Kuznetsov in his paper says "This turns out to be a surprisingly hard problem", and then goes on to use and extend the techniques introduced by Walter in order to solve it.

25.5. The spiral of Theodorus

On May 22, 2003, Walter Gautschi visited us in the Section of Mathematics at the University of Geneva, and gave a colloquium lecture precisely on the topic of the paper [GA**197**]. It was a fascinating lecture, I remember it very well. Like the paper, it started with an intriguing spiral, the spiral of Theodorus, shown in Figure 25.1. As one can see, the spiral is constructed starting at the point $(1,0)$ by always moving in the direction orthogonal to the current position vector, and going precisely a distance of length 1. This gives for the second point $(1,1)$, with a distance $\sqrt{2}$ from the origin (just use Pythagoras), for the third point a location with distance $\sqrt{2+1}$ from the origin (use Pythagoras again), for the fourth point a distance $\sqrt{3+1}$, the

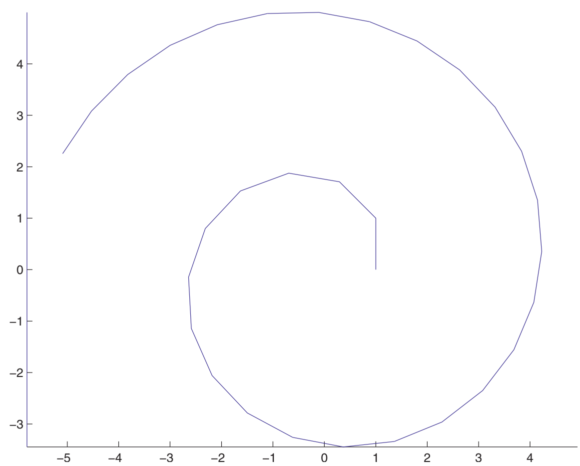

Fig. 25.1. The spiral of Theodorus

general point numbered n having a distance $\sqrt{n}$ from the origin. The distribution of the angles in the spiral of Theodorus has interesting number-theoretic properties (see [4], where the spiral is given the name "Quadratwurzelschnecke"[5]).

Using complex variables, one can also describe this spiral for $\alpha = 1, 2, \ldots$ by the recurrence relation

$$T(\alpha+1) = \left(1 + \frac{i}{\sqrt{\alpha}}\right) T(\alpha), \quad T(1) = 1, \tag{25.2}$$

which gives $T(2) = 1 + i$, $T(3) = (1 + \frac{i}{\sqrt{2}})(1 + i) = 1 - \frac{1}{\sqrt{2}} + i(1 + \frac{1}{\sqrt{2}})$, etc. The spiral of Theodorus is thus obtained by applying a Forward Euler Method (with step 1) to the differential equation

$$T'(\alpha) = \frac{i}{\sqrt{\alpha}} T(\alpha), \tag{25.3}$$

which has as a solution the circle, the dynamics of which, however, slows down more and more as one moves along the circle.

The problem treated by Walter Gautschi, however, is a different one. Professor Davis [1, p. 33ff] had been wondering if it is possible to interpolate the spiral of Theodorus by a smooth, if possible analytic, curve. This problem is similar to a problem Euler faced when he tried to interpolate the factorial function, which led to his discovery of the gamma function. Davis, inspired by Euler's work, found the following interpolant:

$$T(\alpha) = \prod_{k=1}^{\infty} \frac{1 + i/\sqrt{k}}{1 + i/\sqrt{k + \alpha - 1}}, \quad \alpha \geq 0.$$

This product also satisfies the recurrence relation (25.2), and can be evaluated for any value $\alpha \geq 0$. It therefore produces a continuous (in fact, analytic) version of the Theodorus spiral.

Unfortunately, the product is very slowly convergent, and thus not suitable for numerical evaluation. This is where Walter Gautschi comes in: using logarithmic differentiation, he derives a polar representation for the continuous spiral of Theodorus, in which there now appears a slowly convergent series. For a particular point on the spiral (where it crosses the positive real axis for the first time), the series is given by

$$\sum_{k=1}^{\infty} \frac{1}{k^{3/2} + k^{1/2}},$$

the so-called Theodorus constant, and it is with this series that Davis had aroused Walter's interest in this problem. Using again Laplace transforms (cf. Section 25.2), Walter shows how the summation of the series can be transformed into a problem

[5] square-root snail

of integration, which can be solved very effectively by Gaussian quadrature — "an absolute gem of numerical analysis" according to Davis [1, p. 42].

With regard to identifying $T(\alpha)$ in terms of known special functions, however, Davis writes [1, pp. 41/42]: "Computation is one thing, and the identification of $T(\alpha)$ is another matter, and it still eluded me. The Spirit of Euler infused me constantly, but contributed nothing toward the solution. The mistake I made was that I had been consulting the wrong Swiss mathematician. I should have consulted the Swiss-born-and-trained American mathematician, Walter Gautschi, who ... in the course of this work ... also identified $T(\alpha)$."

The analytic Theodorus spiral can also be continued backward into a second sheet of the Riemann surface, as was proposed by J. Waldvogel [6], and Walter concludes with a figure of what he calls the twin-spiral of Theodorus, a very well-chosen name, given the context, and one which I will later also explain to my children.

One could ask what the differential equation might be that describes this twin spiral. It is certainly not equation (25.3), since this one only gives a circle. Something to think about!

25.6. Epilogue

My most recent meeting with Walter Gautschi was at the conference in honor of Claude Brezinski's 70th birthday in Sardinia, in the fall of 2011. As always, we had very nice discussions, Walter and I, and Walter gave a lovely presentation about a real problem from applications [GA**204**], solved in a very elegant way, how could it be different, using Gauss quadrature. I hope we will meet many more times in the future.

References

[1] Philip J. Davis. *Spirals: from Theodorus to chaos*. With contributions by Walter Gautschi and Arieh Iserles. A K Peters, Wellesley, MA, 1993. x+237 pp. ISBN: 1-56881-010-5.

[2] Bernard N. Flury and Gregory Constantine. The F-G diagonalization algorithm. Algorithm AS 211. *Applied Statistics* 34:177–183, 1985

[3] Martin J. Gander and Alan H. Karp. Stable computation of high order Gauss quadrature rules using discretization for measures in radiation transfer. *J. Quantitative Spectroscopy Radiative Transfer*, 68(2):213–223, 2001.

[4] Edmund Hlawka. Gleichverteilung und Quadratwurzelschnecke. *Monatsh. Math.*, 89(1):19–44, 1980. (Excerpted English translation in [1, pp. 157-167].)

[5] A. Kuznetsov. Asymptotic approximations to the Hardy–Littlewood function. *J. Comput. Appl. Math.*, 237(1):603–613, 2013.

[6] Jörg Waldvogel. Analytic continuation of the Theodorus spiral. Preliminary version at *http://www.sam.math.ethz.ch/~waldvoge/Papers/theopaper.html*

Part II

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