PADE APPROXIMANTS AND THEIR APPLICATIONS

edited by
P. R. Graves-Morris

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P. R. GRAVES-MORRIS

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CONTRIBUTORS

F. V. Atkinson, *Mathematics Department, University of Toronto, Canada* (p. 75)

G. A. Baker, Jr., *Applied Mathematics Department, Brookhaven National Laboratory, Upton, New York 11973, U.S.A.* (pp. 83, 147)

D. Bessis, *University of Western Ontario, Canada*, and *Centre d'Etudes Nucleaires de Saclay, France* (p. 275)

J. S. R. Chisholm, *Mathematical Institute, University of Kent, Canterbury, England* (p. 11)

S. C. Chuang, *Department of Computing and Control, Imperial College, University of London, England* (p. 347)

A. K. Common, *Mathematical Institute, University of Kent, Canterbury, England* (p. 201)

H. P. Debart, *C.G.E., Marcoussis, France* (p. 351)

M. E. Fisher, *Baker Laboratory, Cornell University, Ithaca, New York 14850, U.S.A.* (p. 159)

J. Fleischer, *Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87544, U.S.A.* (p. 69)

J. L. Gammel, *Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87544, U.S.A.* (p. 3)

C. R. Garibotti, *Instituto di Fisica dell'Universita, Bari, Italy* (p. 253).

A. C. Genz, *Mathematical Institute, University of Kent, Canterbury, England* (p. 105)

J. Gilewicz, *Centre de Physique Theorique, Marseille, France* (p. 99)

W. B. Gragg, *Mathematics Department, University of California, San Diego, U.S.A.* (p. 117)

P. R. Graves-Morris, *Mathematical Institute, University of Kent, Canterbury, England* (p. 271)

A. J. Guttman, *School of Mathematics, University of Newcastle, Australia* (p. 163)

F. Harbus, *Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, U.S.A.* (pp. 179, 183)

C. Isenberg, *Physics Laboratory, University of Kent, Canterbury, England* (p. 169)

R. C. Johnson, *Mathematics Department, Durham University, Durham, England* (p. 53)

W. B. Jones, *University of Colorado, Boulder, Colorado 80302, U.S.A.* (p. 125)

J. S. Joyce, *Wheatstone Physics Laboratory, Kings College, University of London, England* (p. 163)

A. B. Keats, *Atomic Energy Establishment, Winfrith, Dorset, England* (p. 337)

J. B. Knowles, *Atomic Energy Establishment, Winfrith, Dorset, England* (p. 337)

R. Krasnow, *Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.* (p. 183)

D. Lambeth, *Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, U.S.A.* (p. 183)

D. W. Leggett, *Atomic Energy Establishment, Winfrith, Dorset, England* (p. 337)

L. Lui, *Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, U.S.A.* (p. 183)

C. Lopez, *Universidad Autonoma de Madrid, Spain* (p. 217)

I. M. Longman, *Department of Environmental Sciences, Tel-Aviv University, Israel* (p. 131)

D. Masson, *Department of Mathematics, University of Toronto, Ontario, Canada* (p. 41)

S. Milošević, *Institute of Physics, Belgrade, Yugoslavia* (p. 187)

J. Nuttall, *Physics Department, Texas A & M University, College Station, Texas 77843, U.S.A* and *Physics Department, University of Western Ontario, London, Ontario, Canada* (p. 29)

M. Pusterla, *Istituto de Fisica dell'Universita, Padova, Italy* (p. 299)

J. F. Rennison, *Mathematical Institute, University of Kent, Canterbury, England* (p. 271)

A. Ronveaux, *Facultés Universitaires de Namur, Namur, Belgium* (p. 135)

Y. Shamash, *Department of Computing and Control, Imperial College, University of London, England* (p. 341)

M. I. Sobhy, *Electronics Laboratory, University of Kent, Canterbury, England* (p. 321)

H. E. Stanley, *Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, U.S.A.* (pp. 179, 183)

W. J. Thron, *Department of Mathematics, University of Colorado 80302, U.S.A.* (p. 23)

J. A. Tjon, *Institute for Theoretical Physics, University of Utrecht, The Netherlands* (p. 241)

G. Turchetti, *Istituto di Fisica della Universita, Bologna, Italy* (p. 313)

P. J. S. Watson, *Physics Department, Carleton University, Ottawa, Canada* (p. 93)

F. J. Yndurain, *CERN, Geneva, Switzerland* and *Universidad Autonoma de Madrid, Spain* (p. 217)

V. Zakian, *University of Manchester Institute of Science and Technology, Manchester, England* (p. 141)

Preface

The number of scientific workers who find Padé methods useful in research seems to be growing rapidly. From the original days of the classification of some rational fraction approximants by Padé, no doubt influenced by Hermite at the Ecole Normale Supérieure, and the first theorems of de Montessus, the approximants were viewed as just another form of continued fraction, which was a well established representation. The importance of Padé Approximants as a systematic method of extracting more information from power series expansions occurring so frequently in theoretical physics was stressed by Baker and Gammel in the early 1960's. There has been a steadily growing cross-fertilisation of ideas between analysts, numerical analysts, applied mathematicians, theoretical physicists, theoretical chemists and electrical engineers since then, and this symposium is an attempt to bring together people from these diverse disciplines. The form of the colloquium was a school, primarily instructional, and a conference. The colloquium was completed by the presence of some experts who worked here for a period including both school and conference. This formal framework promoted discussions, appraisal of past work and future projects.

The topics discussed at this conference reflect current progress. The impact of Nuttall's theorem on convergence in measure and the work of the Saclay group on the perturbation series in field theory are two important developments since the publication (also by Academic Press) of "The Padé Approximant in Theoretical Physics", edited by George Baker and John Gammel. For the future, the remark in Prof. Gammel's introductory address, about the difficulties of forming Padé Approximants in several variables, may inspire the development that many of us feel is now within reach.

The conference report is laid out in five sections. The first section contains Prof. Gammel's introductory lecture and the papers on the mathematical properties of Padé Approximants. Second, there are the papers on numerical analysis and algorithms. Third, are the papers on the application of Padé Approximants to critical phenomena etc.. Fourth, come the applications in atomic, nuclear and elementary particle physics and fifth are the papers on circuit synthesis and control. Of course, the work cannot be divided into mutually exclusive sections, and many papers bear on several aspects of applied mathematics in general. The introductory lectures given at the school are being published by the Institute of Physics.

This, the conference book, is published by the camera ready process, which allows rapid publication. For reasons associated with this process, and with the requirement that the book be not too long, contributors were asked to follow some very rigid and seemingly arbitrary rules. Also, a strict length limitation was imposed. I am most grateful to the authors who complied with the instructions. The conference was directed by Prof. J. S. R. Chisholm and Dr. A. K. Common, and Dr. A. K. Common undertook the substantial task of being conference secretary. We are grateful to the Science Research Council, who sponsored the Colloquium, for funds which made the venture possible and to the Institute of Physics under whose auspices the conference was held. I wish to thank John Rennison for his encouragement during the editing, and Profs. L. Fox, J. L. Gammel, J. A. Tjon and J. L. Basdevant for academic advice. We are, as ever, grateful to our secretaries, Sallie Wilkins and Sandra Bateman for their constant and invaluable assistance.

P. R. Graves-Morris

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MATHEMATICAL PROPERTIES OF PADE APPROXIMANTS

REVIEW OF TWO RECENT GENERALIZATIONS OF THE PADÉ APPROXIMANT

J. L. Gammel

(Los Alamos Scientific Laboratory, University of California

Los Alamos, New Mexico 87544, U. S. A.)

1. Quadratic Padé Approximants

The usual Padé approximant to a function $f(z)$ is the ratio of two polynomials, the numerator N of degree n and the denominator D of degree m, defined by

$$Df - N = 0 \quad \text{through} \quad z^{m+n} \quad . \tag{1}$$

In other words, the approximant is the solution of a linear equation.

Recently, R. E. Shafer (1972) of the Lawrence Radiation Laboratory, Livermore, California has suggested that approximants which are the solution of higher order equations may be of value. One sees that if polynomials P of degree p, Q of degree q, and R of degree r are defined by

$$Pf^2 + Qf + R = 0 \quad \text{through} \quad z^{p+q+r+1} \quad , \tag{2}$$

and the (p,q,r) approximant is taken to be an exact root of the quadratic equation, then there is a close analogy with ordinary Padé approximants. These analogies are the following.

First, the equations determining the coefficients in the polynomials P, Q, and R are linear. The power series expansion of $f(z)$ is known; therefore, the power series expansion of

$f^2(z)$ is known, and P, Q, and R, and therefore their coefficients appear in Eq. (2) linearly. Because Eq. (2) is homogeneous, one of the coefficients has to be chosen. Just as the coefficient of z^0 in the denominator of the ordinary Padé approximants is taken to be unity, so the coefficient of z^0 in P may be taken to be unity. Then Eq. (2) yields $p + q + r + 2$ linear equations for the remaining coefficients of Q and R.

Second, the (N, N, N) quadratic approximant is invariant under homographic transformations

$$z = Aw/(1 + Bw) \quad . \tag{3}$$

Let $g(w) = f(Aw/(1 + Bw))$, and let $P_N[f(z)]$ be the (N, N, N) approximant to $f(z)$. Invariance means that

$$P_N[g(w)] = P_N[f(z)]\Big|_{z = \frac{Aw}{1+Bw}} \quad . \tag{4}$$

The proof of this is most easily accomplished by observing that if

$$(p_0 + p_1 z + \ldots + p_N z^N) f^2(z) + (q_0 + q_1 z + \ldots + q_N z^N) f(z)$$
$$+ (r_0 + r_1 z + \ldots + r_N z^N) = 0 \text{ through } z^{3N+1} \quad , \tag{5}$$

then substituting $z = Aw/(1 + Bw)$ and multiplying through by $(1+ Bw)^N$ yields

$$(1 + Bw)^N P\left(\frac{Aw}{1+Bw}\right) g^2(w) + (1 + Bw)^N Q\left(\frac{Aw}{1+Bw}\right) g(w)$$
$$+ (1 + Bw)^N R\left(\frac{Aw}{1+Bw}\right) = 0 \quad \text{through } w^{3N+1} \quad , \tag{6}$$

where the coefficients of g^2, g, and 1 are polynomials of degree N.

Since it is thought that invariance under homographic transformations greatly expands the region of convergence of ordinary [N/N] Padé approximants, so it may be expected that this invariance also greatly expands the region of convergence of (N, N, N) quadratic Padé approximants.

The third property is of importance in physics. This property is that the (N, M, N) Padé approximants to a unitary $f(z)$ (one which satisfies $f(z)f^*(z) = 1$ for z real) are unitary. The proof is pretty and proceeds as follows. By definition,

$$Pf^2 + Qf + R = 0 \quad , \tag{7}$$

and multiplying this by f^{*2} and using $ff^* = 1$,

$$P + Qf^* + Rf^{*2} = 0 \quad . \tag{8}$$

Thus, if

$$f = \frac{-Q - \sqrt{Q^2-4PR}}{2P} \tag{9}$$

is the (N, M, N) quadratic approximant to f, then

$$f^* = \frac{-Q - \sqrt{Q^2-4PR}}{2R} \tag{10}$$

is the (N, M, N) quadratic approximant to f^* . (The equality of the first and last indices is essential at this point: more generally, if Eq. (9) gives the (L, M, N) quadratic approximant to f, Eq. (10) gives the (N, M, L) approximant to f^*. The choice of the opposite sign for the square root is necessitated by the requirement f and f^* both approach unity as $z \to 0$.)

Then clearly,

$$ff^* = 1 \text{ exactly.} \tag{11}$$

It remains to discuss the numerical power of the quadratic approximants, and this power is best illustrated by quadratic approximants to

$$\text{arc tan } z = z - \frac{z^3}{3} + \frac{z^5}{5} \cdots \quad . \tag{12}$$

To get a finite value for arc tan z at $z = \infty$ using ordinary Padé approximants requires some trick such as squaring arc tan z, forming the Padé approximants to the resulting function of z^2, and taking the square root again. Then one obtains

$$\text{arc tan } z = \text{constant} - \frac{\text{constant}'}{z^2} \quad , \text{ as } \quad z \to \infty \quad . \tag{13}$$

This is wrong, because

$$\text{arc tan } z = \text{constant} - \frac{\text{constant}'}{z} \quad , \text{ as } \quad z \to \infty \quad . \tag{14}$$

Shafer's (2, 1, 2) approximant,

$$\text{arc tan } x = \frac{8z}{3 + \sqrt{25 + \frac{80z^2}{3}}} \quad , \tag{15}$$

has the correct behavior at infinity, and it is much better than anything obtained from ordinary Padé approximants using so few terms.

One expects to see much research utilizing Shafer's idea.

2. Approximants Based on Differential Equations

One could go to cubic and quartic Padé approximants, or one might try

$$P_L \frac{df}{dz} + Q_M f + R_N = 0 \quad \text{to order} \quad L + M + N + 1 \ . \qquad (16)$$

Or one might even try second order differential equations, or in fact any sort of non-linear differential equation which one thinks appropriate.

The series related to the theory of critical phenomena should be restudied with these new ideas of Shafer's in mind. In fact, Joyce and Guttmann (1972), having come upon the idea of using second order homogeneous equations in just this way before me and independently of me, have already initiated such a program of work. I shall describe their work in a moment.

Of importance to critical phenomena is the fact that if

$$P \frac{d^n f}{dz^n} + Q \frac{d^{n-1} f}{dz^{n-1}} + \dots = 0 \ , \qquad (17)$$

then the singular points z_c of f are the roots of P. If near a singular point

$$f \simeq \frac{\Gamma}{(z_c - z)^{\alpha}} \ , \qquad (18)$$

then

$$\alpha = 1 - n - \frac{Q(z_c)}{\left.\frac{dP}{dz}\right|_{z=z_c}} \ . \qquad (19)$$

There will be much in these lectures about critical points z_c

and critical indices α. George Baker's trick of taking the logarithmic derivative is equivalent to the homogeneous first order differential equation method.

The expected advantage of such methods is that singularities more complicated than the one shown in Eq. (18) are in fact accommodated exactly. Consider the sum of two such singularities,

$$f = \frac{\Gamma_1}{(z_1-z)^{\alpha_1}} + \frac{\Gamma_2}{(z_2-z)^{\alpha_2}} \quad . \tag{20}$$

Differentiate once,

$$\frac{df}{dz} = \frac{\alpha_1\Gamma_1}{z_1-z}\frac{1}{(z_1-z)^{\alpha_1}} + \frac{\alpha_2\Gamma_2}{z_2-z}\frac{1}{(z_2-z)^{\alpha_2}} \quad . \tag{21}$$

Equations (20) and (21) may be solved for $(z_1-z)^{-\alpha_1}$ and $(z_2-z)^{-\alpha_2}$, (treating $\Gamma_1/(z_1-z)$ as a constant, etc.), and these results substituted into

$$\frac{d^2f}{dz^2} = \frac{\alpha_1(\alpha_1+1)\Gamma_1}{(z_1-z)^2}\frac{1}{(z_1-z)^{\alpha_1}} + \frac{\alpha_2(\alpha_2+1)\Gamma_2}{(z_2-z)^2}\frac{1}{(z_2-z)^{\alpha_2}} \quad , \tag{22}$$

and clearing away denominators one gets a second order linear differential equation with polynomial coefficients.

Combinations of powers and logarithms and powers of logarithms are accommodated: it is only a question of degree of equation and degree of polynomial coefficients required to accommodate any kind of singularities.