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Walter Van Assche (Eds.)

Orthogonal Polynomials and Special Functions

Computation and Applications

Springer

F. Marcellán · W. Van Assche (Eds.)

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Preface

These are the lecture notes of the fifth European summer school on *Orthogonal Polynomials and Special Functions*, which was held at the Universidad Carlos III de Madrid, Leganés, Spain from July 8 to July 18, 2004. Previous summer schools were in Laredo, Spain (2000) [1], Inzell, Germany (2001) [2], Leuven, Belgium (2002) [3] and Coimbra, Portugal (2003) [4]. These summer schools are intended for young researchers preparing a doctorate or Ph.D. and postdocs working in the area of special functions.

For this edition we were happy to have eight invited speakers who gave a series of lectures on a subject for which they are internationally known experts. Seven of these lectures are collected in this volume. The lecture of J. S. Geronimo on *WKB and turning point theory for second order difference equations* has been published elsewhere [5].

The lectures fall into two categories: on one hand we have lectures on *computational aspects* of orthogonal polynomials and special functions and on the other hand we have some modern *applications*. The computational aspects deal with algorithms for computing quantities related to orthogonal polynomials and quadrature (Walter Gautschi's contribution), but recently it was also found that computational aspects of numerical linear algebra are closely related to the asymptotic behavior of (discrete) orthogonal polynomials. The contributions of Andrei Martínez and Bernhard Beckermann deal with this interaction between numerical linear algebra, logarithmic potential theory and asymptotics of discrete orthogonal polynomials. The contribution of Adhemar Bultheel makes the transition between applications (linear prediction of discrete stationary time series) and computational aspects of orthogonal rational functions on the unit circle and their matrix analogues. Other applications in this volume are quantum integrability and separation of variables (Vadim Kuznetsov), the classification of orthogonal polynomials in terms of two linear transformations each tridiagonal with respect to an eigenbasis of the other (Paul Terwilliger), and the theory of nonlinear special functions arising from the Painlevé equations (Peter Clarkson).

Walter Gautschi gave a lecture about *Computational methods and software* for orthogonal polynomials, in particular related to quadrature and approximation. His lecture describes many algorithms which can be used in Matlab. The lecture of Andrei Martínez-Finkelshtein is about *Equilibrium problems of potential theory in the complex plane* and gives a brief introduction to the logarithmic potential in the complex plane and the corresponding equilibrium problems. Minimizing logarithmic energy is very close to best polynomial approximation. In his lecture the equilibrium problem is described in the classical sense, but also the extensions with external fields and with constraints, which are more recent, are considered. The lecture of Bernhard Beckermann on *Discrete orthogonal polynomials and superlinear convergence of Krylov subspace methods in numerical linear algebra* makes heavy use of the equilibrium problem with constraint and external field, which is a necessary ingredient for describing the asymptotics for discrete orthogonal polynomials. This asymptotic behavior gives important insight in the convergence behavior of several numerical methods in linear algebra, such as the conjugate gradient method, the Lanczos method, and in general many Krylov subspace methods.

The contribution of Adhemar Bultheel and his co-authors on *Orthogonal rational functions on the unit circle: from the scalar to the matrix case* extends on one hand the notion of orthogonal polynomials to orthogonal rational functions and on the other hand the typical situation with scalar coefficients to matrix coefficients. The motivation for using orthogonality on the unit circle lies in linear prediction for a discrete stationary time series. The motivation for using rational functions is the rational Krylov method (with shifts) and numerical quadrature of functions with singularities, thereby making the link with the lectures of Gautschi and Beckermann.

Vadim Kuznetsov's lecture on *Orthogonal polynomials and separation of variables* first deals with Chebyshev polynomials and Gegenbauer polynomials, which are important orthogonal polynomials of one variable for which he gives several well known properties. Then he considers polynomials in several variables and shows how they can be factorized and how this is relevant for quantum integrability and separability.

Paul Terwilliger describes *An algebraic approach to the Askey scheme of orthogonal polynomials*. The fundamental object in his contribution is a Leonard pair and a correspondence between Leonard pairs and a class of orthogonal polynomials is given. Even though the description is elementary and uses only linear algebra, it is sufficient to show how the three term recurrence relation, the difference equation, Askey-Wilson duality, and orthogonality can be expressed in a uniform and attractive way using Leonard pairs.

Finally, Peter Clarkson brings us to a very exciting topic: *Painlevé equations — Nonlinear special functions*. The six Painlevé equations, which are nonlinear second-order differential equations, are presented and many important mathematical properties are given: Bäcklund transformations, rational solutions, special function solutions, asymptotic expansions and connection formulae. Several applications of these Painlevé equations are described, such as partial differential equations, combinatorics, and orthogonal polynomials, which brings us back to the central notion in these lecture notes.

We believe that these lecture notes will be useful for all researchers in the field of special functions and orthogonal polynomials since all the contributions contain recent work of the invited speakers, most of which is not available in books or not easily accessible in the scientific literature. All contributions contain exercises so that the reader is encouraged to participate actively. Together with open problems and pointers to the available literature, young researchers looking for a topic for their Ph.D. or recent postdocs looking for new challenges have a useful source for contemporary research problems.

We would like to thank Guillermo López Lagomasino, Jorge Arvesú Carballo, Jorge Sánchez Ruiz, María Isabel Bueno Cachadiña and Roberto Costas Santos for their work in the local organizing committee of the summer school and for their help in hosting 50 participants from Austria, Belarus, Belgium, Denmark, England, France, Poland, Portugal, South Africa, Spain, Tunisia, and the U.S.A. This summer school and these lecture notes and some of the lecturers and participants were supported by INTAS Research Network on Constructive Complex Approximation (03-51-6637) and by the SIAM activity group on *Orthogonal Polynomials and Special Functions*.

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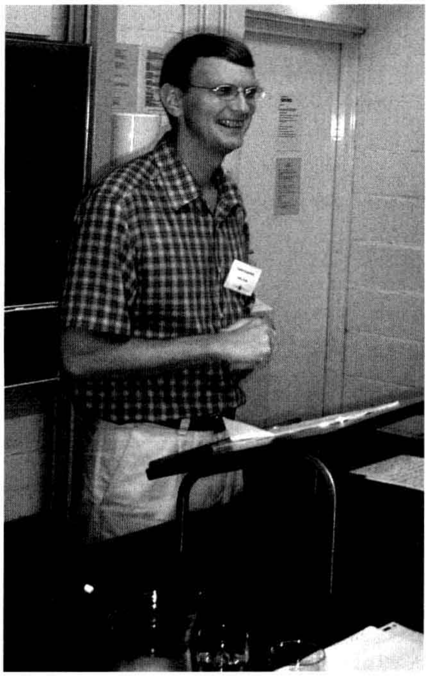
During the processing of this volume we received sad news of the sudden death on December 16, 2005 of Vadim Kuznetsov, one of the contributors. Vadim Kuznetsov enjoyed a very strong international reputation in the field of integrable systems and was responsible for a number of fundamental contributions to the development of separation of variables techniques by exploiting the methods of integrability, a topic on which he lectured during the summer school and which is the subject in his present contribution *Orthogonal polynomials and separation of variables.* We dedicate this volume in memory of Vadim Kuznetsov.



Vadim Kuznetsov 1963–2005

Leganés (Madrid) and Leuven,

Francisco Marcellán
Walter Van Assche

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Orthogonal Polynomials, Quadrature, and Approximation: Computational Methods and Software (in Matlab)

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Summary. One of the main problems in the constructive theory of orthogonal polynomials is the computation of the coefficients, if not known explicitly, in the three-term recurrence relation satisfied by orthogonal polynomials. Two classes of methods are discussed: those based on moment information, and those using discretization of the underlying inner product. Other computational problems considered are the computation of Cauchy integrals of orthogonal polynomials, and the problem of modification, i.e., of ascertaining the effect on the recurrence coefficients of multiplying the weight function by a (positive) rational function. Moment-based methods and discretization algorithms are also available for generating Sobolev orthogonal polynomials, i.e., polynomials orthogonal with respect to an inner product involving derivatives. Of particular interest here is the computation of their zeros.

Important applications of orthogonal polynomials are to the development of quadrature rules of maximum algebraic degree of exactness, most notably Gauss-type quadrature rules, but also Gauss-Kronrod and Gauss-Turán quadratures. Modification algorithms and discretization methods find application to constructing quadrature rules exact not only for polynomials, but also for rational functions with prescribed poles. Gauss-type quadrature rules are applicable also for computing Cauchy principal value integrals. Gaussian quadrature sums are expressible in terms of the related Jacobi matrix, which has interesting applications to generating orthogonal polynomials on several intervals and to the estimation of matrix functionals.

In the realm of approximation, the classical use of orthogonal polynomials, including Sobolev orthogonal polynomials, is to least squares approximation to which interpolatory constraints may be added. Among other uses considered are moment-preserving spline approximation and the summation of slowly convergent series.

All computational methods and applications considered are supported by a software package, called `OPQ`, of Matlab routines which are downloadable individually from the internet. Their use is illustrated throughout.

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1 Introduction

Orthogonal polynomials, unless they are classical, require special techniques for their computation. One of the central problems is to generate the coefficients in the basic three-term recurrence relation they are known to satisfy. There are two general approaches for doing this: methods based on moment information, and discretization methods. In the former, one develops algorithms that take as input given moments, or modified moments, of the underlying measure and produce as output the desired recurrence coefficients. In theory, these algorithms yield exact answers. In practice, owing to rounding errors, the results are potentially inaccurate depending on the numerical condition of the mapping from the given moments (or modified moments) to the recurrence coefficients. A study of related condition numbers is therefore of practical interest. In contrast to moment-based algorithms, discretization methods are basically approximate methods: one approximates the underlying inner product by a discrete inner product and takes the recurrence coefficients of the corresponding discrete orthogonal polynomials to approximate those of the desired orthogonal polynomials. Finding discretizations that yield satisfactory rates of convergence requires a certain amount of skill and creativity on the part of the user, although general-purpose discretizations are available if all else fails.

Other interesting problems have as objective the computation of new orthogonal polynomials out of old ones. If the measure of the new orthogonal polynomials is the measure of the old ones multiplied by a rational function, one talks about modification of orthogonal polynomials and modification algorithms that carry out the transition from the old to the new orthogonal polynomials. This enters into a circle of ideas already investigated by Christoffel in the 1850s, but effective algorithms have been obtained only very recently. They require the computation of Cauchy integrals of orthogonal polynomials — another interesting computational problem.

In the 1960s, a new type of orthogonal polynomials emerged — the so-called Sobolev orthogonal polynomials — which are based on inner products involving derivatives. Although they present their own computational challenges, moment-based algorithms and discretization methods are still two of the main working tools. The computation of zeros of Sobolev orthogonal polynomials is of particular interest in practice.

An important application of orthogonal polynomials is to quadrature, specifically quadrature rules of the highest algebraic degree of exactness. Foremost among them is the Gaussian quadrature rule and its close relatives, the Gauss–Radau and Gauss–Lobatto rules. More recent extensions are due to Kronrod, who inserts $n+1$ new nodes into a given n-point Gauss formula, again optimally with respect to degree of exactness, and to Turán, who allows derivative terms to appear in the quadrature sum. When integrating functions having poles outside the interval of integration, quadrature rules of polynomial/rational degree of exactness are of interest. Poles inside the interval of integration give rise to Cauchy principal value integrals, which pose computational problems of their own. Interpreting Gaussian quadrature sums in terms of matrices allows interesting applications to orthogonal polynomials on several intervals, and to the computation of matrix functionals.

In the realm of approximation, orthogonal polynomials, especially discrete ones, find use in curve fitting, e.g. in the least squares approximation of discrete data. This indeed is the problem in which orthogonal polynomials (in substance if not in name) first appeared in the 1850s in work of Chebyshev. The presence of interpolatory constraints can be handled by a modification algorithm relative to special quadratic factors. Sobolev orthogonal polynomials also had their origin in least squares approximation, when one tries to fit simultaneously functions together with some of their derivatives. Physically motivated are approximations by spline functions that preserve as many moments as possible. Interestingly, these also are related to orthogonal polynomials via Gauss and generalized Gauss-type quadrature formulae. Slowly convergent series whose sum can be expressed as a definite integral naturally invite the application of Gauss-type quadratures to speed up their convergence. An example are series whose general term is expressible in terms of the Laplace transform or its derivative of a known function. Such series occur prominently in plate contact problems.

A comprehensive package, called `OPQ`, of Matlab routines is available that can be used to work with orthogonal polynomials. It resides at the web site

`http://www.cs.purdue.edu/archives/2002/wxg/codes/`

and all its routines are downloadable individually.

2 Orthogonal Polynomials

2.1 Recurrence Coefficients

Background and Notation

Orthogonality is defined with respect to an inner product, which in turn involves a measure of integration, $\mathrm{d}\lambda$. An *absolutely continuous* measure has the form

$$\mathrm{d}\lambda(t) = w(t)\mathrm{d}t \quad \text{on } [a,b], \qquad -\infty \le a < b \le \infty,$$

where w is referred to as a *weight function*. Usually, w is positive on (a,b), in which case $\mathrm{d}\lambda$ is said to be a *positive measure* and $[a,b]$ is called the *support* of $\mathrm{d}\lambda$. A *discrete measure* has the form

$$\mathrm{d}\lambda_N(t) = \sum_{k=1}^{N} w_k \delta(t - x_k)\mathrm{d}t, \qquad x_1 < x_2 < \cdots < x_N,$$

where δ is the Dirac delta function, and usually $w_k > 0$. The support of $\mathrm{d}\lambda_N$ consists of its N *support points* $x_1, x_2, \ldots, x_N$. For absolutely continuous measures, we make the standing assumption that all *moments*

$$\mu_r = \int_{\mathbb{R}} t^r \mathrm{d}\lambda(t), \qquad r = 0, 1, 2, \ldots,$$

exist and are finite. The *inner product* of two polynomials p and q relative to the measure $\mathrm{d}\lambda$ is then well defined by

$$(p,q)_{\mathrm{d}\lambda} = \int_{\mathbb{R}} p(t)q(t)\mathrm{d}\lambda(t),$$

and the *norm* of a polynomial p by

$$\|p\|_{\mathrm{d}\lambda} = \sqrt{(p,p)_{\mathrm{d}\lambda}}.$$