Methods of Computer Algebra for Orthogonal Polynomials

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Rutgers Experimental Mathematics Seminar January, 30, 2014 / Rutgers University

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Online Demonstrations with Computer Algebra

Computer Algebra Systems

 I will use the computer algebra system Maple to program and demonstrate the considered methods.

Algorithms

The mostly used algorithms are:

- Algorithms of Linear Algebra with many variables
- Multivariate polynomial factorization
- and the solution of non-linear systems of polynomial equations.

Orthogonal Polynomials

Scalar Products

Given: a scalar product

$$\langle f,g \rangle := \int_{\alpha}^{\beta} f(x)g(x) \, d\mu(x)$$

with non-negative Borel measure $\mu(x)$ supported in the interval $[\alpha, \beta]$ (or equivalently as a Riemann-Stieltjes integral with nondecreasing $\mu(x)$).

Special Cases

- absolutely continuous measure $d\mu(x) = \rho(x) dx$ with weight function $\rho(x)$,
- discrete measure $\mu(x) = \rho(x)$ supported in \mathbb{Z} .

Orthogonality

• A system of polynomials $(P_n(x))_{n\geq 0}$ with $\deg(P_n)=n$

$$P_n(x) = k_n x^n + k'_n x^{n-1} + k''_n x^{n-2} + \cdots, \quad k_n \neq 0$$

is called orthogonal (OPS) w. r. t. the positive-definite measure $\mu(x)$, if

$$\langle P_m, P_n \rangle = \begin{cases} 0 & \text{if } m \neq n \\ h_n > 0 & \text{if } m = n \end{cases}$$

General Properties of OPS

Main Properties

• (Three-term Recurrence) Every OPS satisfies

$$x P_n(x) = a_n P_{n+1}(x) + b_n P_n(x) + c_n P_{n-1}(x)$$
.

- (Zeros) All zeros of an OPS are simple, lie in the interior of $[\alpha, \beta]$ and have some nice interlacing properties.
- (Representation by Moments)

$$P_{n}(x) = C_{n} \begin{vmatrix} \mu_{0} & \mu_{1} & \cdots & \mu_{n} \\ \mu_{1} & \mu_{2} & \cdots & \mu_{n+1} \\ \vdots & \vdots & \vdots & \vdots \\ \mu_{n-1} & \mu_{n+1} & \cdots & \mu_{2n-1} \\ 1 & x & \cdots & x^{n} \end{vmatrix},$$

where $\mu_n := \int_{\alpha}^{\beta} x^n d\mu(x)$ denote the moments of $d\mu(x)$.

Classical Families

Classical "Continuous" Families

The classical OPS $(P_n(x))_{n\geq 0}$ can be defined as the polynomial solutions of the differential equation:

$$\sigma(x)P_n''(x) + \tau(x)P_n'(x) - \lambda_n P_n(x) = 0.$$

Conclusions

• The coefficient of
$$x^n$$

yields
$$\tau(x) = dx + e, d \neq 0$$

yields
$$\sigma(x) = ax^2 + bx + c$$

yields
$$\lambda_n = n(a(n-1) + d)$$

Classical Families

Classification

These classical families can be classified (modulo linear transformations) according to the following scheme (Bochner (1929))

$$\bullet$$
 $\sigma(x)=0$

$$\bullet$$
 $\sigma(x) = 1$

$$\bullet$$
 $\sigma(x) = x$

•
$$\sigma(x) = 1 - x^2$$

$$\bullet$$
 $\sigma(x) = x^2$

powers xⁿ

Hermite polynomials

Laguerre polynomials

Jacobi polynomials

Bessel polynomials

Ingredients

For the theory one needs

- a representing family $f_n(x)$, here the powers $f_n(x) = x^n$,
- an operator, here the derivative operator D, with the simple property $D f_n(x) = n f_{n-1}(x)$.



Hermite, Laguerre, Jacobi and Bessel

Classical Families

Pearson Differential Equation

The corresponding weight function $\rho(x)$ satisfies the Pearson Differential Equation

$$\frac{d}{dx}\Big(\sigma(x)\rho(x)\Big)=\tau(x)\rho(x).$$

Weight Function

Hence it is given by

$$\rho(x) = \frac{C}{\sigma(x)} e^{\int \frac{\tau(x)}{\sigma(x)} dx} .$$

Classical Continuous Families

The following properties are equivalent, each defining the classical continuous families.

- Differential equation for $(P_n(x))_{n\geq 0}$.
- Pearson Differential Equation $(\sigma \rho)' = \tau \rho$ for weight $\rho(x)$.
- With $(P_n(x))_{n\geq 0}$ also $(P'_{n+1}(x))_{n\geq 0}$ is an OPS.
- Derivative Rule:

$$\sigma(x) P'_n(x) = \alpha_n P_{n+1}(x) + \beta_n P_n(x) + \gamma_n P_{n-1}(x).$$

• Structure Relation: $P_n(x)$ satisfies

$$P_n(x) = \widehat{a}_n P'_{n+1}(x) + \widehat{b}_n P'_n(x) + \widehat{c}_n P'_{n-1}(x)$$
.

• Rodrigues Formula: $P_n(x)$ is given as

$$P_n(x) = \frac{E_n}{\rho(x)} \frac{d^n}{dx^n} \Big(\rho(x) \, \sigma(x)^n \Big) \ .$$

Classical Discrete Families

Classical Discrete OPS

- By replacing the differential operator D by the difference operator $\Delta f(x) = f(x+1) f(x)$ one gets a rather similar theory for the classical discrete OPS that are solutions of certain difference equations.
- In this case the representing family are the falling factorials $f_n(x) = x^{\underline{n}} = x(x-1)\cdots(x-n+1)$ with the property $\Delta f_n(x) = n f_{n-1}(x)$.
- The classification leads to the Charlier, Meixner, Krawtchouk and Hahn polynomials.
- Both the continuous and the discrete classical OPS can be represented by hypergeometric functions.

Hypergeometric Functions

Generalized Hypergeometric Function

The formal power series

$$_{p}F_{q}\left(\begin{array}{c}a_{1},\ldots,a_{p}\\b_{1},\ldots,b_{q}\end{array}\middle|z\right)=\sum_{k=0}^{\infty}A_{k}\,z^{k}\;,$$

whose summands $\alpha_k = A_k z^k$ have a rational term ratio

$$\frac{\alpha_{k+1}}{\alpha_k} = \frac{A_{k+1} z^{k+1}}{A_k z^k} = \frac{(k+a_1) \cdots (k+a_p)}{(k+b_1) \cdots (k+b_q)} \frac{z}{(k+1)} ,$$

is called the generalized hypergeometric function.

Hypergeometric Functions

Hypergeometric Terms

The summand $\alpha_k = A_k z^k$ of a hypergeometric series is called a hypergeometric term.

Formula for Hypergeometric Terms

For the coefficients of the generalized hypergeometric function one gets the following formula using the shifted factorial (Pochhammer symbol) $(a)_k = a(a+1)\cdots(a+k-1)$

$$_{p}F_{q}\left(\begin{array}{c}a_{1},\ldots,a_{p}\\b_{1},\ldots,b_{q}\end{array}\middle|z\right)=\sum_{k=0}^{\infty}\frac{(a_{1})_{k}\cdots(a_{p})_{k}}{(b_{1})_{k}\cdots(b_{q})_{k}}\frac{z^{k}}{k!}$$

Hypergeometric Functions

OPS as Hypergeometric Functions

- Substituting the power series $f(x) = \sum_{k=0}^{\infty} A_k x^k$ into the differential equation and equating coefficients yields a recurrence equation for A_k .
- Using this recurrence one gets for example for the Laguerre polynomials

$$L_n^{\alpha}(x) = \binom{n+\alpha}{n} {}_1F_1 \binom{-n}{\alpha+1} x = \sum_{k=0}^n \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} x^k,$$

and the Hahn polynomials are given by

$$Q_n^{(\alpha,\beta)}(x,N) = {}_3F_2\left(\begin{array}{c|c} -n,-x,n+1+\alpha+\beta & 1 \\ \alpha+1,-N & 1 \end{array}\right).$$

Properties of Classical OPS

Relations Between Classical OPS

Using linear algebra one can compute the coefficients of the following identities – expressed through the parameters a, b, c, d und e - (Lesky (1985), K./Schmersau (1998)):

(RE)
$$x P_n(x) = a_n P_{n+1}(x) + b_n P_n(x) + c_n P_{n-1}(x)$$

(DR)
$$\sigma(x) P'_n(x) = \alpha_n P_{n+1}(x) + \beta_n P_n(x) + \gamma_n P_{n-1}(x)$$

(SR)
$$P_n(x) = \hat{a}_n P'_{n+1}(x) + \hat{b}_n P'_n(x) + \hat{c}_n P'_{n-1}(x)$$

Maple

Classical OPS Solutions of Holonomic Recurrence Equations

Inverse Algorithm

- We showed that the coefficients of the recurrence equation of the classical systems can be written in terms of the coefficients a, b, c, d, and e of the differential / difference equation.
- If one uses these formulas in the backward direction, then one can determine the possible differential / difference equations from a given recurrence.
- For this purpose one must solve a non-linear system.

Classical OPS Solutions of Holonomic Recurrence Equations

Example

Given: the recurrence equation

$$P_{n+2}(x) - (x-n-1) P_{n+1}(x) + \alpha(n+1)^2 P_n(x) = 0$$

Does this equation have classical OPS solutions? *Maple*

• We find out that the solutions of this equation are shifted Laguerre polynomials for $\alpha = 1/4$. For $\alpha < 1/4$ the recurrence has Meixner and Krawtchouk polynomial solutions.

Zeilberger Algorithm

Recurrence Equations for Hypergeometric Series

Doron Zeilberger (1990) designed an algorithm to compute recurrence equations for hypergeometric sums of the type

$$s_n = \sum_{k=-\infty}^{\infty} F(n,k) .$$

Holonomic Recurrence Equations

His algorithm results in a holonomic recurrence equation for s_n . A recurrence equation is called holonomic if it is linear, homogeneous, and has polynomial coefficients.



Doron Zeilberger

Zeilberger Algorithm

Differential Equations for Hypergeometric Series

A similar algorithm yields a holonomic differential equation for series of the form

$$s(x) = \sum_{k=-\infty}^{\infty} F(x,k) .$$

Algebra of Holonomic Differential resp. Recurrence Equations

 Holonomic functions form an algebra, i. e. sum and product of holonomic functions are again holonomic, and there are linear algebra algorithms to determine the resulting differential and recurrence equations.

Zeilberger Algorithm

Application to Orthogonal Polynomials

 As an example, we will apply Zeilberger's algorithm to the Laguerre polynomials

$$L_n^{\alpha}(x) = \sum_{k=0}^n \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} x^k.$$

• With the above algorithms one can also compute recurrence and differential equations for the square $L_n^{\alpha}(x)^2$, or for the difference $L_{n+1}^{\alpha}(x) - L_n^{\alpha}(x)$.

Maple

Power Series Algorithm

Inverse Algorithm

• Whereas Zeilberger's algorithm uses the right hand side of

$$f(x) = \sum_{k=-\infty}^{\infty} A_k x^k$$

to detect its left hand side (or a differential equation for it), my FPS algorithm (= Formal Power Series) starts from the left hand side to detect the right hand side.

 This algorithm (K. (1992)) has been embedded in Maple by Torsten Sprenger as

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convert(...,FormalPowerSeries).
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Maple

Online Orthogonal Polynomials

CAOP = Computer Algebra and Orthogonal Polynomials

- CAOP is a web tool for calculating formulas for orthogonal polynomials belonging to the Askey-Wilson scheme using Maple.
- The implementation of CAOP was originally done by René Swarttouw as part of the Askey-Wilson Scheme Project performed at RIACA in Eindhoven in 2004.
- The present site is a completely revised version of this project which has been done by Torsten Sprenger under my supervision in 2012 and is maintained at the University of Kassel.
- http://www.caop.org/

Askey-Wilson Scheme

Askey-Wilson Scheme

- In CAOP you saw all the families of the Askey-Wilson Scheme.
- Besides the already mentioned cases there are the
 - discrete measure supported in $q^{\mathbb{Z}}$ (Hahn tableau);
 - discrete measure supported on a quadratic lattice (Wilson tableau);
 - discrete measure supported on a q-quadratic lattice (Askey-Wilson tableau).
- It turns out that the three above classes can be treated in a similar way as the continuous and the discrete cases leading to similar theories.
- However, these computations are very tedious and can be done much easier with the use of computer algebra. This research is ongoing and not yet finished.

I would like to thank you very much for your interest!