Computer Algebra Methods for Orthogonal Polynomials

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Online Demonstrations with Computer Algebra

- I will use the computer algebra system *Maple* to demonstrate and program the algorithms presented.
- Of course, we could also easily use any other general purpose system like *Mathematica*, MuPAD or Reduce.
- The following algorithms are most prominently used (internally): linear algebra techniques, multivariate polynomial factorization and the solution of nonlinear equations, e. g. by Gröbner basis techniques.

An Appetizer

- As an appetizer we consider the conversion between a recurrence equation and a difference equation.
- In this talk a difference equation is an equation involving the forward difference operator
$$\Delta f(x) = f(x+1) - f(x)\ .$$
- Question: How can one convert a recurrence equation
$$a_p\, f(x+p) + \cdots + a_1\, f(x+1) + a_0\, f(x) = 0$$
(involving the shift operator) to a difference equation (involving the forward difference operator)? *Maple*

Scalar Products

- Given: a scalar product

$$\langle f, g \rangle := \int_a^b f(x)g(x)\, d\mu(x)$$

with non-negative Borel measure $\mu(x)$ supported in an interval $[a, b]$.

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

Orthogonal Polynomials

- A family $P_n(x)$ of polynomials

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

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

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

Classical Families

- The classical orthogonal polynomials 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:
  - $n = 1$ implies $\tau(x) = dx + e, d \neq 0$
  - $n = 2$ implies $\sigma(x) = ax^2 + bx + c$
  - coefficient of x^n implies $\lambda_n = -n(a(n-1) + d)$

Classification

- The classical systems can be classified according to the following scheme (Bochner 1929):

- $\sigma(x) = 0$ powers x^n
- $\sigma(x) = 1$ Hermite polynomials
- $\sigma(x) = x$ Laguerre polynomials
- $\sigma(x) = x^2$ powers, Bessel polynomials
- $\sigma(x) = x^2 - 1$ Jacobi polynomials

 

 

Hermite, Laguerre, Jacobi and Bessel

Weight function

- The weight function $\rho(x)$ corresponding to the differential equation satisfies Pearson's differential equation

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

- Hence it is given as

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

Classical Discrete Families

- The classical "discrete" orthogonal polynomials can be defined as the polynomial solutions of the difference equation: $(\nabla f(x) = f(x) - f(x-1))$

$$\sigma(x)\Delta\nabla P_n(x) + \tau(x)\Delta P_n(x) + \lambda_n P_n(x) = 0\,.$$

- Conclusions:
  - $n = 1$ implies $\tau(x) = dx + e, d \neq 0$
  - $n = 2$ implies $\sigma(x) = ax^2 + bx + c$
  - coefficient of x^n implies $\lambda_n = -n(a(n-1) + d)$

Classification

- The classical discrete systems can be classified according to the scheme (Nikiforov, Suslov, Uvarov 1991):
- $\sigma(x) = 0$ — falling factorials $x^{\underline{n}} = x(x-1)\cdots(x-n+1)$
- $\sigma(x) = 1$ — translated Charlier polynomials
- $\sigma(x) = x$ — falling factorials, Charlier, Meixner, Krawtchouk polynomials
- $\deg(\sigma(x), x) = 2$ — Hahn polynomials

Sergei Suslov

Weight function

- The weight function $\rho(x)$ corresponding to the difference equation satisfies Pearson's difference equation

$$\Delta\Big(\sigma(x)\rho(x)\Big) = \tau(x)\rho(x) \; .$$

- Hence it is given by

$$\frac{\rho(x+1)}{\rho(x)} = \frac{\sigma(x)+\tau(x)}{\sigma(x+1)} \; .$$

Hypergeometric Functions

- The power series

$$ {}_pF_q\left(\begin{matrix} a_1, \ldots, a_p \\ b_1, \ldots, b_q \end{matrix} \middle| \, z \right) = \sum_{k=0}^{\infty} A_k \, z^k \; , $$

whose summands $\alpha_k = A_k z^k$ have 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 Terms

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

- The relation

$$\frac{\rho(x+1)}{\rho(x)} = \frac{\sigma(x)+\tau(x)}{\sigma(x+1)}$$

therefore states that the weight functions $\rho(x)$ of classical discrete orthogonal polynomials are hypergeometric terms w. r. t. the variable x.

Formula for Hypergeometric Terms

- For the coefficients of the hypergeometric function one gets the formula

$$
{}_pF_q\left(\left.\begin{matrix} a_1, \ldots, a_p \\ b_1, \ldots, b_q \end{matrix}\right| z\right) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_p)_k}{(b_1)_k \cdots (b_q)_k} \frac{z^k}{k!} \,,
$$

in terms of the Pochhammer symbol (or shifted factorial)

$$
(a)_k = a(a+1)\cdots(a+k-1) = \frac{\Gamma(a+k)}{\Gamma(a)} \,.
$$

Classical Orthogonal Polynomials of Hahn Class as Hypergeometric Functions

- From the differential or difference equation, one can determine a hypergeometric representation. *Maple*
- One gets, for example, for the Laguerre polynomials

$$L_n^{\alpha}(x) = \binom{n+\alpha}{n} \, {}_1F_1\left(\left.\begin{matrix} -n \\ \alpha+1 \end{matrix}\right| x\right) = \sum_{k=0}^{n} \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} x^n ,$$

and the Hahn polynomials are given by

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

Properties of Classical Discrete Orthogonal Polynomials

- Moreover, by linear algebra one can determine the coefficients of the following identities

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

(DR) $$\sigma(x)\,\Delta P_n(x) = \alpha_n\,P_{n+1}(x) + \beta_n\,P_n(x) + \gamma_n\,P_{n-1}(x)$$

(SR) $$P_n(x) = \widehat{a}_n\,\Delta P_{n+1}(x) + \widehat{b}_n\,\Delta P_n(x) + \widehat{c}_n\,\Delta P_{n-1}(x)$$

in terms of the given numbers a, b, c, d and e. *Maple*

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Zeilberger's Algorithm

- Doron Zeilberger (1990) developed an algorithm to detect a holonomic recurrence equation for hypergeometric sums

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

- A recurrence equation is called holonomic, if it is homogeneous, linear and has polynomial coefficients.

Zeilberger's Algorithm

- A similar algorithm detects a holonomic differential equation for sums of the form

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

- Holonomic functions form an algebra, i.e. sum and product of holonomic functions are holonomic, and there are linear algebra algorithms to compute the corresponding differential / recurrence equations.

Application to Orthogonal Polynomials

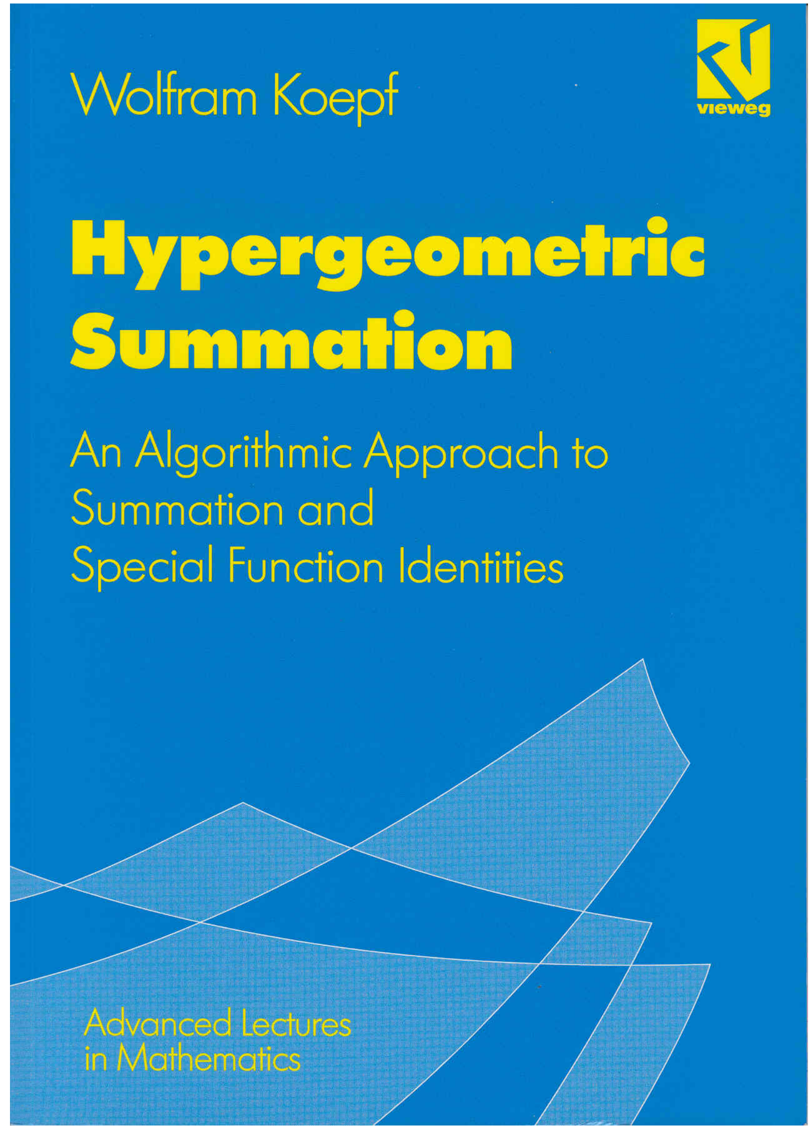
- As an example, we apply Zeilberger's algorithm to the Laguerre polynomials

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

- Using the holonomic algebra, it is also easy to find recurrence and differential equations for the square $L_n^\alpha(x)^2$ and for the product $L_n^\alpha(x)\, L_m^\beta(x)$. Maple

The software used was developed for my book

Hypergeometric Summation, Vieweg, 1998, Braunschweig/Wiesbaden



and can be downloaded from my home page:

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Petkovsek-van Hoeij Algorithm

- Marko Petkovsek (1992) developed an algorithm to find all hypergeometric term solutions of a holonomic recurrence equation.
- This algorithm is not very efficient, but finishes the problem to find hypergeometric term representations of hypergeometric sums $s_n = \sum\limits_{k=-\infty}^{\infty} F(n,k)$ like $\sum\limits_{k=0}^{n} \binom{n}{k}^2$ algorithmically.
- Mark van Hoeij (1999) gave a very efficient version of such an algorithm, and implemented it in Maple.

Recurrence Operators

- Assume we consider the holonomic recurrence equation

$$R\, f(x) := f(x+2) - (x+1)\, f(x+1) + x^2\, f(x) = 0\ .$$

- In the general setting the coefficients could be rational functions w.r.t. x.

- Let τ denote the shift operator $\tau\, f(x) = f(x+1)$. Then the above recurrence equation can be rewritten as $R\, f(x) = 0$ with the operator polynomial

$$R := \tau^2 - (x+1)\,\tau + x^2\ .$$

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Recurrence Operators

- Such operators form a non-commutative algebra.
- The product rule for the shift operator

$$\tau\Big(x\,f(x)\Big) = (x+1)\,f(x+1) = (x+1)\,\tau\,f(x)$$

is equivalent to the commutator rule

$$\tau\,x - x\,\tau = \tau$$

in this algebra.

Some Facts

- An operator polynomial has a first order right factor iff the recurrence has a hypergeometric term solution.
- Hence Petkovsek's algorithm finds first order right factors of operator polynomials.
- Multiplying an operator polynomial from the left by a rational function in x is equivalent to multiply the recurrence equation by this rational function.
- Multiplying an operator polynomial from the left by τ is equivalent to substitute x by $x+1$ in the recurrence equation.

Construction of Fourth Order Recurrence

- Let us construct a fourth-order recurrence equation.
- To construct the equation $S\,f(x) = 0$ with operator

$$S := (x\,(x+1)\tau^2 + x^3\,\tau + (x^2+x-1)) \cdot R\ ,$$

we just add the equations

$$(x^2+x-1)\left(f(x+2) - (x+1)\,f(x+1) + x^2\,f(x)\right) = 0$$

$$x^3\left(f(x+3) - (x+2)\,f(x+2) + (x+1)^2\,f(x+1)\right) = 0$$

$$x\,(x+1)\left(f(x+4) - (x+3)\,f(x+3) + (x+2)^2\,f(x+2)\right) = 0\ .$$

Factorization of Recurrence Equations

- This leads to

$$
\begin{aligned}
S \;:=\; & x\,(x+1)\,\tau^4 \\
& -x\,(4\,x+3)\,\tau^3 \\
& +(x+1)\left(3\,x^2+6\,x-1\right)\tau^2 \\
& +(x+1)\left(x^4+x^3-x^2-x+1\right)\tau \\
& +\left(x^2+x-1\right)x^2\,.
\end{aligned}
$$

- Given S, a factorization procedure by Mark van Hoeij can compute the factorization $S = L\,R$, again.

Classical Orthogonal Polynomial Solutions of Recurrence Equations

- Previously we had shown how the recurrence equation can be explicitly expressed in terms of the coefficients of the differential / difference equation.
- If one uses this information in the opposite direction, then the corresponding differential / difference equation can be obtained from a given three-term recurrence.

Example

- Let the recurrence

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

be given.

- We can compute that for $\alpha = 1/4$ this corresponds to translated Laguerre polynomials, and for $\alpha < 1/4$ Meixner and Krawtchouk polynomial solutions occur.

The End

Thank you very much for your attention!