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 system like *Mathematica*, MuPAD or Reduce.

• The following algorithms are most prominently used: linear algebra techniques, multivariate polynomial factorization and the solution of nonlinear equations, e.g. by Gröbner basis techniques.
Scalar Products

• Given: a scalar product

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

with non-negative 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 $\mathbb{Z}$,
  – discrete measure $\mu(x) = \rho(x)$ with support in $q^{\mathbb{Z}}$. 
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

$$\langle P_m, P_n \rangle = \begin{cases} 
0 & \text{if } m \neq n \\
\frac{d_n^2}{n} & \text{if } m = n
\end{cases}$$
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 scheme (Bochner 1929):
  - $\sigma(x) = 0$ \hspace{1cm} powers $x^n$
  - $\sigma(x) = 1$ \hspace{1cm} Hermite polynomials
  - $\sigma(x) = x$ \hspace{1cm} Laguerre polynomials
  - $\sigma(x) = x^2$ \hspace{1cm} powers, Bessel polynomials
  - $\sigma(x) = x^2 - 1$ \hspace{1cm} Jacobi polynomials
Hermite, Laguerre, Jacobi and Bessel
Weight function

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

\[
\frac{d}{dx} \left( \sigma(x) \rho(x) \right) = \tau(x) \rho(x).
\]

- 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: $(\Delta f(x) = f(x + 1) - f(x), \nabla f(x) = f(x) - f(x - 1))$

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

- 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
    \[ x^n = x(x - 1) \cdots (x - n + 1) \]
  - $\sigma(x) = 1$ translated Charlier polynomials
  - $\sigma(x) = x$ falling factorials, Charlier, Meixner, Krawtchouk polynomials
  - $\deg(\sigma(x), x) = 2$ Hahn polynomials
Weight function

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

\[
\Delta \left( \sigma(x) \rho(x) \right) = \tau(x) \rho(x).
\]

- Hence it is given as

\[
\frac{\rho(x + 1)}{\rho(x)} = \frac{\sigma(x) + \tau(x)}{\sigma(x + 1)}.
\]
Hypergeometric Functions

- The power series

\[ pF_q \left( \begin{array}{c} a_1, \ldots, a_p \\ b_1, \ldots, b_q \end{array} \bigg| z \right) = \sum_{k=0}^{\infty} A_k z^k, \]

whose coefficients \( \alpha_k = A_k z^k \) 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 $x$. 
Coefficients of Hypergeometric Functions

- For the coefficients of the hypergeometric function we get the formula

\[ pFq\left(\begin{array}{c}
{a_1, \ldots, a_p} \\
{b_1, \ldots, b_q}
\end{array} \bigg| z\right) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_p)_k \cdot \cdots \cdot (b_q)_k \cdot z^k}{(b_1)_k \cdots (b_q)_k \cdot k!}, \]

where \((a)_k = a(a + 1) \cdots (a + k - 1)\) is called the Pochhammer symbol (or shifted factorial).
Examples of Hypergeometric Functions

\[ e^z = {}_0F_0(z) \]

\[ \sin z = z \cdot {}_0F_1\left(\frac{-}{3/2} \middle| -\frac{z^2}{4}\right) \]

- Further examples: \( \cos(z), \arcsin(z), \arctan(z), \ln(1 + z), \text{erf}(z), L_n^{(\alpha)}(z), \ldots \), but for example not \( \tan(z) \).
Classical Discrete Orthogonal Polynomials of Hahn Class as Hypergeometric Functions

From the differential or difference equation, one can determine a hypergeometric representation.

To get this representation, one determines by linear algebra the coefficients of the following identities

\begin{align*}
\text{(RE)} \quad x P_n(x) &= a_n P_{n+1}(x) + b_n P_n(x) + c_n P_{n-1}(x) \\
\text{(DR)} \quad \sigma(x) P'_n(x) &= \alpha_n P_{n+1}(x) + \beta_n P_n(x) + \gamma_n P_{n-1}(x) \\
\text{(SR)} \quad P_n(x) &= \hat{a}_n P'_{n+1}(x) + \hat{b}_n P'_n(x) + \hat{c}_n P'_{n-1}(x)
\end{align*}

in terms of the given numbers \( a, b, c, d \) and \( e \).
Combining these equations one obtains for the coefficients $C_k(n)$ of the power series for the monic polynomials

$$\tilde{P}_n(x) = \sum_{k=0}^{n} C_k(n) x^n$$

(again by linear algebra) the recurrence equation

$$(k - n)(an + d - a + ak)C_k(n)$$

$$+(k + 1)(bk + e)C_{k+1}(n)$$

$$+c(k + 1)(k + 2)C_{k+2}(n) = 0.$$
Classical Discrete Orthogonal Polynomials of Hahn Class as Hypergeometric Functions

- From these general results, we get, for example, for the Laguerre polynomials

\[ L_n^\alpha(x) = \frac{(\alpha + 1)_n}{n!} \, _1F_1\left( \begin{array}{c} -n \\ \alpha + 1 \end{array} \middle| x \right), \]

and the Hahn polynomials are given by

\[ h_n^{(\alpha, \beta)}(x, N) = \frac{(-1)^n(N - n)_n(\beta + 1)_n}{n!} \, _3F_2\left( \begin{array}{c} -n, -x, \alpha + \beta + n + 1 \\ \beta + 1, 1 - N \end{array} \middle| 1 \right). \]
Zeilberger’s Algorithm

• In 1990 Zeilberger 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.

• The holonomic recurrence equation constitutes a normal form for holonomic sequences.
Zeilberger’s Algorithm

- A similar algorithm detects a holonomic differential equation for sums of the form
  \[ s(x) = \sum_{k=-\infty}^{\infty} F(x, k) . \]
- The holonomic differential equation constitutes a normal form for holonomic functions.
- 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 examples, we apply Zeilberger’s algorithm to the Laguerre polynomials

\[ L_\alpha^n(x) = \frac{(\alpha + 1)_n}{n!} \binom{-n}{\alpha + 1} \binom{x}{1} \]

and to the Hahn polynomials \( h_{n,\alpha,\beta}(x, N) = \]

\[ \frac{(-1)^n(N - n)_n(\beta + 1)_n}{n!} \binom{-n,-x,\alpha + \beta + n + 1}{\beta + 1,1 - N} \binom{1}{1}. \]
The software used was developed for my book

Hypergeometric Summation, Vieweg, 1998, Braunschweig/Wiesbaden

and can be downloaded from my home page:

http://www.mathematik.uni-kassel.de/~koepf
Computation of the Differential Equation from the Recurrence Equation

- We have 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!