A MACSYMA Package for the Generation and Manipulation of Chebyshev Series (Extended Abstract)

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1. Summary

Techniques for a MACSYMA package for expanding an arbitrary univariate expression as a truncated series in Chebyshev polynomials and manipulating such expansions is described. A data structure is introduced to represent a truncated expansion in a set of orthogonal polynomials. The data structure contains the independent variable, the name of the orthogonal polynomial set, the number of terms retained, and a list of the expansion coefficients. Although we restrict attention here to the set of Chebyshev polynomials as the orthogonal set, extension to other orthogonal polynomials will be done later. A data structure for truncated power series is provided as an alternative.

The principal function of the package converts a given expression into the aforementioned data structure. Special cases are the conversion of sums, products, the ratio, or the composition of truncated Chebyshev expansions.

Another special case is converting an expression free of truncated Chebyshev expansions. The package generates exact expansion coefficients whenever possible. In addition to well-known Chebyshev expansions, such as for polynomials, we provide new methods for getting exact Chebyshev expansions for reciprocals of polynomials of degree one or two, meromorphic functions, arbitrary powers of a first-degree polynomial, the error-function, and generalized hypergeometric functions .

When exact Chebyshev expansions for a function are unknown, or too costly to compute, approximate expansions are performed. Conversion to power series and interpolation between the roots of a Chebyshev polynomial are supported. The Clenshaw method for symbolic Chebyshev expansion of the solution of a linear differential equation whose coefficients are low degree polynomials is implemented in the package.

2. Data Structure

Orthogonal polynomials are generalizations of perpendicular vectors. The perpendicularity of vectors **a**, **b** with components a(i), b(i), namely $\sum a(i)b(i) = 0$, is generalized to polynomial functions a(x), b(x) of continuous variates x by a generalized perpendicularity, $\int w(x)a(x)b(x)\,dx = 0$. Here w(x) is a weight function. Orthogonal polynomials arise in the solution of some problems in mathematical physics [1], and a symbolic package for their error-free manipulation is beneficial to workers in that field.

The truncated expansion in a set of univariate orthogonal polynomials named *orthpoly* is represented by the data structure:

orthser(*indep_var*, *coefficient_list*, *orthpoly*,
desc(*highest_index_of_exact_coefficient*,
highest_index_of nonzero_coeff))

where *indep_var* is the argument of the orthogonal polynomial and *coefficient_list* is a MACSYMA list of expansion coefficients.

We call such a data structure an **orthser** and provide functions for converting any expression into an orthser, in particular an orthser whose *indep_var* is atomic. The resulting orthser can be inexact, not only due to truncating at a finite number of terms but also due to the coefficients themselves being inexact. Even simple conversions, such as for the product of two orthsers, can contaminate coefficients. All items in *coefficient_list* with index less than or equal to the first argument of **desc** are exact.

In this paper the orthogonal polynomial set is restricted to the set of Chebyshev polynomials:

$T_n(x) = \cos(n \cos^{-1}(x))$ (2–1)

[2], which are representative of general orthogonal polynomials but have a simpler calculus. Chebyshev expansions are also useful in providing close to the best supnorm approximations of functions by polynomials [3][11].

In later work we will consider other orthogonal polynomials and convert from one set of orthogonal polynomials to another, corresponding to a change of basis in the vector space of polynomials. This is done through the intermediary of the basis of powers of the independent variable.

3. Conversion to a Truncated Series in Orthogonal Polynomials

Expressions which are converted to an orthser (with atomic *indep_var*) are one of these types:

1] linear combination, product, or ratio of orthsers,

2] expression containing no orthsers

3] linear combination, product, or ratio of types 1 and 2

4] orthser whose *indep_var* is an orthser

5] univariate expression whose argument is an orthser, **f(orthser(,,,))**

6] orthser whose *indep_var* is a univariate function whose argument is one of the previous types.

Of these, type 6 can be reduced to type 4 or 5 by converting the *indep_var* or argument to an orthser. Similarly type 3 can be reduced to 1 or 2. Expressions of type 5 can be reduced to type 4 by converting f(a*x) to **orthser(x,,,)** using the rules of 2 and substituting the orthser argument of f for x/a. The multiplier a is chosen to keep x of absolute value less than 1, to improve the rate of convergence of the Chebyshev series.

A linear combination of orthsers with the same *indep_var* reduces to an orthser with the appropriate linear combination of the *coefficient_lists* . A product of two Chebyshev orthsers is reduced to a single orthser by using the rule:

$$T_m(x)\, T_n(x) = \frac{1}{2}\left(T_{m+n}(x)+T_{|m-n|}(x)\right) \quad (3\text{–}1)$$

[4] and the distributive law. Because this rule is so simple, it is cheaper to calculate the product within the Chebyshev polynomial basis and avoid back and forth interconversion with the power basis.

Type 4 is a composition of Chebyshev series. It can be converted to a single orthser by conversion to the power basis, doing the composition in the power basis, and converting back to the Chebyshev basis. An alternative calculation of Chebyshev series composition avoids conversion to the power basis by reducing composition to multiplication and addition of orthsers. Let

$$S_M = \sum_{m=0}^{M} \alpha_m T_m(X) \quad (3\text{–}2)$$

where

$$X = \sum_{m=0}^{M} \beta_m T_m(x) \quad (3\text{–}3)$$

We seek S_M as a single Chebyshev series in x. The three-term recurrence for Chebyshev polynomials with adjacent indices can be written in matrix-vector form [5]:

$$\begin{bmatrix} T_{n+1}(X) \\ T_n(X) \end{bmatrix} = A.\begin{bmatrix} T_n(X) \\ T_{n-1}(X) \end{bmatrix} \quad (3\text{–}4)$$

where

$$A(X) = \begin{bmatrix} 2X & -1 \\ 1 & 0 \end{bmatrix} \quad (3\text{–}5)$$

Then S_M can be written :

$$S_M = \alpha_0 T_0(x) + \text{first}\left(S^{(1)}.\begin{bmatrix} T_1(x) \\ T_0(x) \end{bmatrix}\right) \quad (3\text{–}6)$$

where $S^{(1)}$ is the matrix polynomial:

$$S^{(1)} = \sum_{k=1}^{M} \alpha_k A^{k-1}$$

and first takes the first component of a vector. The Horner form of $S^{(1)}$ yields a recurrence which produces $S^{(1)}$ solely in terms of sums and products of two orthsers.

$$v^{[M,0]} = \alpha_M \begin{bmatrix} X \\ 1 \end{bmatrix} \quad (3\text{–}7)$$

$$v^{[M,i]} = (\alpha_M \mathbf{I} + A(X)) \,.\, v^{[M,i-1]}(\mathbf{X}) \quad i=1,\ldots,M-1$$

$$S_M = \alpha_0 + \text{first}\left(v^{[M,M-1]}(\mathbf{X})\right)$$

This method generalizes to all other orthogonal polynomials, which also have three-term recurrences for polynomials with adjacent indices.

4. Conversion of Expressions Containing No Orthsers

We seek the Chebyshev expansion coefficients, A_m, of g(x):

$$g(x) = \sum_{m=0}^{\infty} A_m\, T_m(x) \quad (4\text{-}1)$$

and truncate the list of A_m at some value m to produce the coefficient_list of the orthser. When g depends on parameters, we seek a symbolic expression for A_m, exact if possible.

4.1 Exact Chebyshev Expansion Coefficients

Although in principle one could get an exact A_m from the mutual orthogonality of Chebyshev polynomials

$$A_m = \frac{2}{\pi(1+\delta_{0m})}\int_{-1}^{1} \frac{g(x)T_m(x)}{\sqrt{1-x^2}}\,dx \quad (4.1\text{-}1)$$

we relegate this alternative to a user option, since we expect that in general a symbolic definite integral package will fail to give an answer, even after much effort. Instead we derive some special methods for exact Chebyshev expansion coefficients, which are invoked by pattern matching of g. Should these fail, approximate methods for A_m are used.

4.1.1 Application of the Bessel Function Generator

The generating function for modified Bessel functions can be put into the form of a Chebyshev expansion [6]:

$$\exp(a\,x) = 2\sum_{n=0}^{\infty}{}' I_n(a)\,T_n(x) \quad (4.1.1\text{-}1)$$

where $|x|<=1$ and the prime on the summation means that its first term is halved. From this expansion, Chebyshev expansions can be obtained, not only for the exponential, but also for sin(ax), cos(ax), sinh(ax),cosh(ax). A slightly more complicated application of (4.1.1–1) is

$$\mathrm{erf}(ax) = \frac{a}{\sqrt{\pi}}\exp\left(-\frac{a^2}{2}\right)\sum_{m=0}^{\infty} (-)^m \frac{I_m(a)+I_{m+1}(a)}{2m+1} T_{2m+1}(x) \quad (4.1.1\text{-}2)$$

4.1.2 The Chebyshev Transform Lemma and Its Applications

For an independent variable x, let

$$x_+ = x + \sqrt{x^2-1} \quad (4.1.2\text{-}1a)$$
$$x_- = x - \sqrt{x^2-1} \quad (4.1.2\text{-}1b)$$

We define the Chebyshev transform of f(x) to be

$$F(x) = \frac{1}{2}\left(f(x_+)+f(x_-)\right) \quad (4.1.2\text{-}2)$$

It is easy to show that the Chebyshev transform of x^n is $T_n(x)$ [7], from which follows the

Lemma The expansion coefficients of the Maclaurin expansion of f(x) are identically the Chebyshev expansion coefficients of its Chebyshev transform F(x).

To apply this lemma to the Chebyshev expansion coefficients of F(x), one would, in principle, find the inverse transform f(x) and expand f in Maclaurin series. Instead of inverting the Chebyshev transform using a Poisson integral formula [10], we guess a form for f and take the Chebyshev transform, hoping that the resulting F is simple and interesting. What simplify F are the identities:

$$x_+ + x_- = 2x \quad (4.1.2\text{-}3)$$
$$x_+ * x_- = 1 \quad (4.2.2\text{-}4)$$

For example, if f(x)=1/(1-Qx), then up to scaling constants F(x)=1/(1-qx), where $|q|<1$ and

$$Q(q) = \frac{q}{1+\sqrt{1-q^2}} \quad (4.1.2\text{-}5)$$

so that F(x) has the Chebyshev expansion[12]:

$$\frac{1}{1-qx} = \frac{2}{\sqrt{1-q^2}}\sum_{n=0}^{\infty}{}' Q^n\,T_n(x) \quad (4.1.2\text{-}6)$$

Choosing f(x) = $\tanh^{-1}(x)$ yields F(x)=(1/2) $\tanh^{-1}(x)$ so that

$$\tanh^{-1}(x) = 2\sum_{n=0}^{\infty}{}' \frac{1}{2n+1} T_n(x) \quad (4.1.2\text{-}7)$$

Similarly choosing f(x) = $\tan^{-1}(a\,x)$ yields the expansion

$$\tan^{-1}(q\,x) = 2\sum_{n=0}^{\infty}{}' \frac{(-Q)^{2n+1}}{2n+1} T_n(x) \quad (4.1.2\text{-}8)$$

and choosing f(x)=ln(1-ax) yields

$$\ln(1-qx) = -\ln(1-Q^2) + 2\sum_{n=1}^{\infty}{}' \frac{Q^n}{n} T_n(x) \quad (4.1.2\text{-}9)$$

In all the above examples, f and F had similar structure. The ratio of two polynomials exhibits the same behavior. If f is a polynomial of degree n-1 divided by a polynomial of degree n, then so is F, except for an additive constant. This can be used to derive the Chebyshev expansion of the ratio of a linear to a quadratic in x. It turns out that one can solve relations between the parameters with no greater effort than solving a quadratic equation in a parameter.

A more complicated application of the Chebyshev transform lemma gives the Chebyshev expansion coefficients of $\sqrt{(1-qx)}$ as the Maclaurin expansion coefficients of:

$$\sqrt{1+2(1-qx)-\sqrt{4-4qx+q^2}} \quad (4.1.2\text{-}10)$$

4.1.3 Chebyshev Expansion of Rational and Meromorphic Functions

If the denominator of a rational function $M(x):=N(x)/D(x)$ can be factored into linear and quadratic factors with real coefficients, then a partial fraction expansion reduces the rational function to a sum of terms, each of which can be treated by a method in the previous section. Repeated factors of D(x) can be treated by appropriate differentiation with respect to a parameter. Should any of the roots of D should lie in the interval [-1, 1], one should avoid Chebyshev expansion of the term in the partial fraction expansion containing that root.

If the coefficients of powers of x in D are all numeric, then numeric factorization of D is possible using the MACSYMA function **allroots.**

Meromorphic functions are generalizations of rational functions, in which N and D are not polynomials but power series. Chebyshev expansions for N/D can be derived when the roots of D, possibly infinite in number, are known. We consider the special case of N/D bounded at infinity and all roots of D, i.e. all poles of the meromorphic function M(x), being simple. Then M, as a function of the complex variable z, has a well-known partial fraction expansion [8]:

$$M(z) = M(0) + \sum_{j=1}^{\infty} b_j\left(\frac{1}{z-a_j} + \frac{1}{a_j}\right) \quad (4.1.3\text{–}1)$$

where a_j is the j^{th} pole of M and b_j is the residue of M at a_j. Specializing further to M(z) real for real z and poles either real, a_j, or pure imaginary, $i\, s_n$:

$$M(x) = M_0+M_1(x)+xM_2(x)+M_3(x) \quad (4.1.3\text{–}2)$$

where

$$M_1(x) = \sum_{j=1}^{\infty} \frac{b_j}{z-a_j} \quad (4.1.3\text{–}3)$$

$$M_2(x) = \sum_{n=0}^{\infty} \frac{\sigma_n}{x^2+s_n^2} \quad (4.1.3\text{–}4)$$

$$M_3(x) = \sum_{n=0}^{\infty} \frac{\tau_n}{x^2+s_n^2} \quad (4.1.3\text{–}5)$$

$$M_0 = M(0)+\sum_{j=1}^{\infty} \frac{b_j}{a_j} - \sum_{n=0}^{\infty} \frac{\tau_n}{s_n} \quad (4.1.3\text{–}6)$$

where σ_n and τ_n are 2 times the real part and -2 times the imaginary part of the residue of M at $i\, s_n$, respectively. Each of the terms of M_1, M_2, M_3 can be expanded in Chebyshev series using (4.1.2–6). (Note that, although $|a_j|$ should exceed 1, s_n can be arbitrarily small, i.e. poles can lie on the imaginary axis arbitrarily close to the origin.) The resulting coefficient of a $T_m(x)$ becomes an infinite sum of the m^{th} powers of various Q, one Q for each pole.

Chebyshev expansions for tan(αx) and sec(αx), where poles are evenly spaced, were obtained using this method. For m>3 convergence of the infinite sum in the coefficient of T_m was sufficiently rapid to be truncated at ten terms for a relative error of 10^{-8}. For smaller m, the entire series was summed using truncated Maclaurin expansions in α, whose coefficients involve Bernoulli or Euler numbers.

4.1.4 Miscellaneous Exact Expansions

Expansion (4.1.1–1) yields the expansion:

$$(1-qx)^{-\alpha} = 2{\sum_{l=0}^{\infty}}' T_l(x)\, G_l(\alpha,q) \quad (4.1.4\text{–}1)$$

where

$$G_m(\alpha,q) = \left(\frac{q}{2}\right)^m \frac{1}{m\, B(\alpha,m)}\, {}_2F_1\left(\alpha,\ \alpha+m,\ m+1, \frac{1-\sqrt{1-q^2}}{1+\sqrt{1-q^2}}\right) \quad (4.1.4\text{–}2)$$

B is the beta function, and ${}_2F_1$ is the hypergeometric function. For q=1, where the series form of the hypergeometric function diverges, a special method gives the expansion coefficients of $(1-x)^{-\alpha}$ in terms of a recurrence.

Calculating the hypergeometric series motivates a Chebyshev economization, and we can get the exact Chebyshev expansion coefficients of the hypergeometric series in terms of other hypergeometric functions. In general, the k^{th} exact Chebyshev expansion coefficient for the generalized hypergeometric function ${}_sF_t$ (**a**; **b**; qx) is proportional to

$$q^k\, {}_{2s}F_{2t+1}\left(\frac{\mathbf{a}+\mathbf{k}^{\langle s\rangle}}{2}, \frac{\mathbf{a}+\mathbf{k}^{\langle s\rangle}+\mathbf{1}^{\langle s\rangle}}{2}; \frac{\mathbf{b}+\mathbf{k}^{\langle t\rangle}}{2}, \frac{\mathbf{b}+\mathbf{k}^{\langle t\rangle}+\mathbf{1}^{\langle t\rangle}}{2}, k+1; \left(2^{s+1}q\right)^2\right)$$

where **a** is a vector of s components, **b** is a vector of t components, and $\mathbf{k}^{<s>}$ is a vector of s components all equal to k.

4.2 Approximate Chebyshev Expansion Coefficients

When the exact Chebyshev expansion coefficients cannot be obtained by the above methods, the following methods are available for approximate expansion coefficients.

1] Expanding the expression as a Maclaurin series in x to a large number of terms and converting the resulting polynomial to a truncated Chebyshev series.

2) Interpolating at the roots of a Chebyshev polynomial [3].

Should the expression y(x) to be expanded satisfy a linear differential equation with coefficients of the derivatives appearing as a polynomials in x of low order and with appropriate initial conditions, the expansion can be obtained by a symbolic implementation of the Clenshaw method [9]. The highest derivative of y appearing in the differential equation is expanded as a truncated Chebyshev series with unknown coefficients. Successively lower derivatives are obtained, also as truncated Chebyshev expansions, using the relation [3]:

$$\int T_m(x)\,dx = \left(\frac{1}{2}\right)\left(\frac{T_{m+1}(x)}{m+1} - \frac{T_{|m-1|}(x)}{m-1}\right) + K \qquad (4.2\text{–}1)$$

The polynomial coefficients of the derivatives are also expanded as truncated Chebyshev series, appropriate series are multiplied and substituted in the differential equation. Coefficients of corresponding Chebyshev polynomials are equated. The resulting equations and equations in the unknown coefficients resulting from the initial conditions are solved for the unknown coefficients.

5. Conclusions

Procedures in a package for generating exact Chebyshev expansion coefficients for many functions have been described. In addition to well-known Chebyshev expansions, such as for polynomials, we provided new methods for getting exact Chebyshev expansions for reciprocals of polynomials of degree one or two, meromorphic functions, arbitrary powers of a first-degree polynomial, the error-function, and generalized hypergeometric functions.

When exact Chebyshev expansions for a function are unknown, or too costly to compute, approximate expansions were performed.

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[1] See, for example, H. Margenau and Murphy "The Mathematics of Physics and Chemistry" Van Nostrand

[2] This expression can be shown to be a polynomial in x by showing from the definition that $T_0(x)=1$, $T_1(x)=x$, and (the recurrence) $T_{n+1}(x)=2xT_n(x)-T_{n-1}(x)$. From the recurrence it follows that T_{n+1} is a polynomial in x if T_n and T_{n-1} are.

[3] E. Cheney "Introduction to Approximation Theory" Second Ed. Chelsea New York 1982 p126

[4] L. Fox and I. Parker "Chebyshev Polynomials in Numerical Analysis" Oxford London 1968

[5] Massachusetts Institute of Technology, Artificial Intelligence Laboratory AI Memo 239, a.k.a.*Hakmem*

[6] M. Abramowitz and I. Stegun "Handbook of Mathematical Functions" National Bureau of Standards AMS 55 Washington 1964. p376,(9.6.34)

[7] The identity $x_+^n + x_-^n = 2\,T_n(x)$ appears in M. Snyder "Chebyshev Methods in Numerical Approximation" Prentice-Hall Englewood Cliffs, New Jersey 1966 p13, (1.1–14) as an alternative definition of T_n but not as part of a Chebyshev transform.

[8] E. Whittaker and G. Watson "A Course in Modern Analysis" Third Ed. Cambridge 1920 p134

[9] C. Clenshaw "Chebyshev Series for Mathematical Functions" Her Majesty's Stationery Office London 1962, See also K. Geddes 1977 MACSYMA users' conference.

[10] We didn't know that there was an exact form for the inverse of the Chebyshev transform until W. Kahan taught us that the inverse can be obtained by a Poisson integral. In fact:

$$f(x) = \frac{1}{2\pi i}\int_\Gamma F\left(\frac{1}{2}(w+1/w)\right)\left(\frac{w+x}{w-x}\right)\frac{dw}{w}$$

where the integration contour is a unit circle, and F(x) is real. He learned it from J.C.P. Miller at Cambridge in the mid 1950's. The appropriate Poisson integral formula is given in [G. Carrier, M. Krook, and C. Pearson "Theory of Functions of a Complex Variable", McGraw-Hill, 1966, p.47] We know of no case where using the Poisson integral formula gives an answer that could not be obtained by guessing at the inverse. For the case of (4.1.2-6), guessing the inverse Chebyshev transform is much simpler than calculating the Poisson integral by residues. The residue method requires calculating the location of poles, determining whether they are

inside the contour, and calculating the residue of those that lie inside. Moreover, the residue method must invoke analytic continuation in the case of complex q.

[11] The advantage of Chebyshev approximations can be glimpsed by comparing numerical approximations for e. The exact value is 2.718...; truncating the Maclaurin series for e^x at $O(x^4)$ yields 2.708; the corresponding (2,2)Pade approximant is 2.714; truncating the Chebyshev series at $O(T_4(x))$ yields 2.718.

[12] In the seminal paper on Chebyshev series: C.Lanczos, J.Math. & Phys. 17,123(1938), eq. (4.1.2-6) is derived in a different way. A three-term recurrence with constant coefficients is solved, using as a boundary condition the vanishing of all coefficients in the Chebyshev series witrh index beyond a fixed n. The index n is then allowed to go to infinity. Characteristically, truncating Chebyshev series at a finite index n gives more complicated answers than do the exact Chebyshev series.