Chebyshev Polynomials: After the Spelling the Rest is Easy

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CHEBYSHEV POLYNOMIALS: AFTER THE SPELLING THE REST IS EASY

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Chebyshev polynomials, although seldom encountered by physicists in their formal training, have a wide variety of practical uses in numerical algorithms and are easy to compute and apply. Being orthogonal polynomials, they share many properties with the familiar Legendre polynomials, but are generally much better behaved. As orthogonal basis functions, Chebyshev polynomials are related to Fourier cosine functions and to Fourier series, with the advantage that they are polynomials rather than the infinite series defining the cosine. In the physical sciences Chebyshev polynomials are therefore applied to a wide variety of computing problems—such as parametrizing null geodesics for rotating black holes,[1] evaluating two-electron Gaussian integrals in computational chemistry,[2] calculating radiative properties of hydrogenic systems for describing opacities of stellar envelopes,[3] and solving numerically the Navier–Stokes differential equations for unsteady flows in cavities.[4]

In this column I give an introduction to properties and applications of Chebyshev polynomials that are useful for numerical applications in physics, along with a few algorithms. Because these polynomials are relatively unfamiliar to physicists, I provide more background than usual. The topics discussed are analytical properties, the minimax criterion, curve fitting and interpolation, economization of series, and numerical differentiation and integration.

What's in a name?

Mathematician Pafnuty Lvovich Chebyshev (1821–94) spent most of his career at Petersburg University in Russia, where he made significant contributions to engineering mechanics, artillery ballistics, probability theory, and the stability of equilibrium (he was a colleague of Lyapunov). In the late 1870s, he invented a calculating machine—minimal justification for describing his work in this journal. Transliteration of the Cyrillic spelling of his name into various European languages has been confusingly variable—you may meet Chebyshev, Tchebichiev, Tschebyscheff, Tchebychef, and Čebyšev—but with the first spelling gradually predominating. Perhaps this variability of spelling has discouraged use of Chebyshev (etc.) polynomials by physicists, although mathematicians use them extensively in formal work.

Let us summarize some properties of these interesting polynomials. The Chebyshev polynomial of the first kind, degree n ($n=0,1,2,\ldots$), and argument x (usually assumed to be real and bounded by ± 1) is $T_n(x)$, defined by

$$T_n(x) \equiv \cos(n\theta), \quad \theta = \arccos x. \tag{1}$$

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For general n, these relations provide as good a way as any to compute numerical values of T_n accurately and efficiently. To use T_n with a variable t in the finite range $[a, b]$, we make the mapping into the range $[-1, 1]$ of x by the linear transformation

$$x = \frac{2t-(b+a)}{b-a}. \tag{2}$$

Various nonlinear transformations can be used if t is unbounded from below ($a \to -\infty$) or from above ($b \to \infty$). We assume henceforth that the x range is $[-1, 1]$. The formulas for cosines of multiples of angles ensure that T_n is a *polynomial* in x of order n.

Figure 1 provides a novel visualization of Eq. (1) in terms of projecting points onto a line describing uniform circular motion, so that the T_n are also discrete points along a line for a particle undergoing simple harmonic motion. This property relates Chebyshev expansions to Fourier series expansions, with $n-1$ corresponding to the order of the harmonic and $n=1$ being the fundamental, as is clear from the figure. The functions in Eq. (1) are usually just called the Chebyshev polynomials, although there are polynomials of the second kind and analogous polynomials defined over different ranges of x, as discussed in Beckmann's practical text on orthogonal polynomials.[5] For example, the polynomials of the second kind are $U_n(x)$, defined by

$$U_n(x) \equiv \sin[(n+1)\theta]/\sin\theta, \quad \theta = \arccos x,$$
$$= \frac{1}{n+1}\frac{dT_{n+1}(x)}{dx} \tag{3}$$

for $n=0,1,\ldots$. Except near the end points $x=\pm 1$, numerical values of U_n can be computed accurately from the defining relations. Near the end points, Taylor expansions can be made about the extremum values $U_n(\pm 1) = \pm(n+1)$.

A quick way to generate formulas and graphs for T_n and U_n is to use a programming system such as MAPLE[6] or MATHEMATICA.[7] Box 1 shows a simple program for these Chebyshev polynomials from $n=0$ to 6, written in MAPLE V, Release 2. (Our column in the next issue is a detailed comparison of MAPLE and MATHEMATICA.) Since as n increases the magnitude of $U_n(x)$ becomes large as $n \to \pm 1$, its graph is shown only for $|x| < 0.9$. Generally, $U_n(x)$ is less used in practical applications than is $T_n(x)$, which is bounded by ± 1, as seen in the upper graph in Box 1. Notice that $T_n(-0.5) = -0.5$, unless n is divisible by 3, when $T_n(-0.5) = 1$, as is easily derived from Eq. (1). Since the $T_n(x)$ are cosines, their size varies between ± 1 for any n, unlike the Legendre polynomials, whose use T_n can often displace, which attain these values only at the end points and whose other extrema gradually decrease in magnitude as the order increases. Unlike Legendre polynomials, which have zero derivatives at the end points, in the neighborhood of $x = \pm 1$, T_n varies with increasing rapidity as n increases, as is clear from

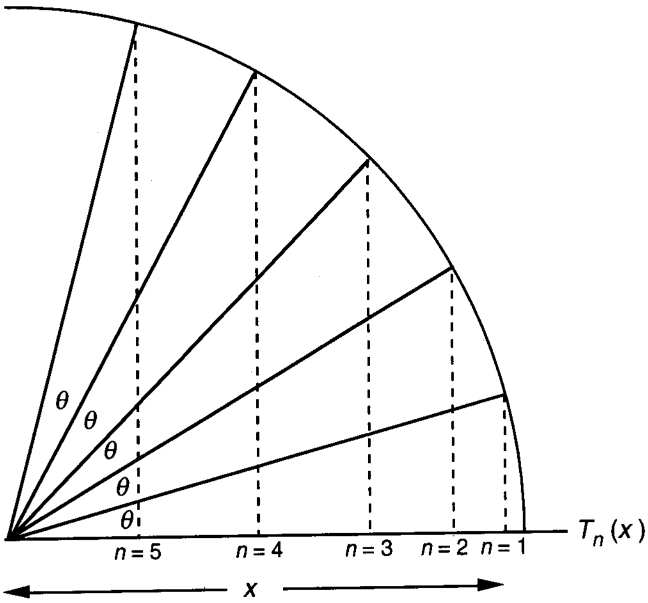


Figure 1. According to Eq. (1), $T_n(x)$ is the projection onto the $\theta=0$ axis of a point on the unit circle at angle $n\theta$, with $\theta=\arccos x$. Note that $T_1(x)=x$.

the upper graphic in Box 1 or from the second relation in Eq. (3) combined with the extremum values of U_n.

Many algebraic properties of the Chebyshev polynomials are derived in Chap. 1 of Rivlin's monograph,[8] and a summary of their properties is tabulated in Chap. 22 of Abramowitz and Stegun,[9] mixed in with those of the other orthogonal polynomials, which is sometimes awkward. To generate $T_n(x)$ we can use the recurrence relation

$$T_{n+1}(x)=2xT_n(x)-T_{n-1}(x), \quad n>1, \qquad T_1(x)=x, \quad T_0(x)=1. \tag{4}$$

Notice that the parity of $T_n(x)$ is $(-1)^n$, which is also apparent if we express powers of x in terms of Chebyshev polynomials, such as:

$$\begin{aligned} &x^0=T_0, \quad x^1=T_1, \quad x^2=1/2(T_0+T_2),\\ &x^3=1/4(3T_1+T_3), \quad x^4=1/8(3T_0+4T_2+T_4),\\ &x^5=1/16(10T_1+5T_3+T_5),\\ &x^6=1/32(10T_0+15T_2+6T_4+T_6). \end{aligned} \tag{5}$$

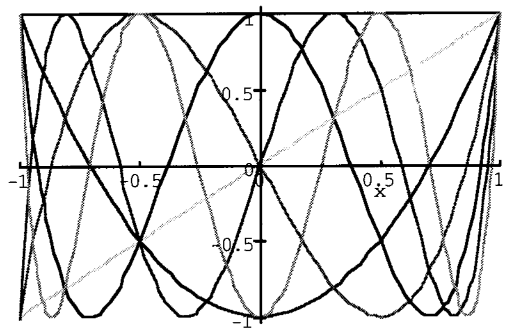
In x^n the highest-order polynomial $T_n(x)$ appears with the lowest weight, $1/2^{n-1}$, a result that is particularly useful for discussing economization of series, as we do below. Explicit expressions for powers up to x^{12} given in Table 22.3 in Abramowitz and Stegun[9] are examples of the general expression derived as follows:

Box 1. MAPLE program and output for the first seven Chebyshev polynomials T_n and U_n. The graphical outputs were pasted from separate windows. Each degree n can be identified by noting that T_n and U_n have n zeros in $[-1,1]$.

```
> # Chebyshev polynomials
> interface(prettyprint=2) # superscripts
> with(orthopoly,T,U):
> print(`Tn(x) & Un(x): (n>=0,-1<=x<=1)`):
                    Tn(x) & Un(x): (n>=0, -1<=x<=1)
> ChebyT := seq(eval(T(n,x)),n=0..6);
```

$$ChebyT := 1,\ x,\ 2x^2-1,\ 4x^3-3x,\ 8x^4-8x^2+1,\ 16x^5-20x^3+5x,\ 32x^6-48x^4+18x^2-1$$

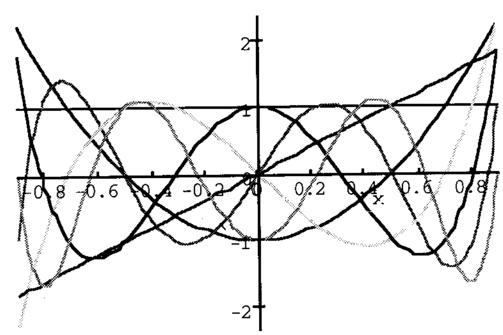
```
> plot({ChebyT},x=-1..1); # to plot T
```




```
> ChebyU := seq(eval(U(n,x)),n=0..6);
```

$$ChebyU := 1,\ 2x,\ 4x^2-1,\ 8x^3-4x,\ 16x^4-12x^2+1,\ 32x^5-32x^3+6x,\ 64x^6-80x^4+24x^2-1$$

```
> plot({ChebyU},x=-0.9..0.9); # to plot U
```



$$\begin{aligned} x^k=\cos^k\theta&=\left(\frac{e^{i\theta}+e^{-i\theta}}{2}\right)^k\\ &=\frac{1}{2^{k-1}}\left\{\cos[k\theta]+\binom{k}{1}\cos[(k-2)\theta]+\binom{k}{2}\right.\\ &\quad\left.\times\cos[(k-4)\theta]+\cdots\right\}\\ &=\frac{1}{2^{k-1}}\left[T_k(x)+\binom{k}{1}T_{k-2}(x)+\binom{k}{2}T_{k-4}(x)+\cdots\right] \end{aligned} \tag{6}$$

in which one takes half the binomial coefficient of T_0 if k is even. The second line in this equation follows by applying the binomial expansion to the previous expression and collecting terms.

Applications of orthogonal polynomials, such as Gaussian integration, often require knowing their zeros—typically a messy calculation, as for the Legendre polynomials. The zeros of Chebyshev polynomials can be written down by inspection of Eq. (1), namely $T_n(x)$ has n zeros, given by x_{0i}, where

$$x_{0i}=\cos\left(\frac{\pi(i-1/2)}{n}\right), \quad i=1,2,\ldots,n. \tag{7}$$

Formulas for locating the extrema of $T_n(x)$ are similarly simple, and the extreme values are ± 1.

Orthogonality relations of Chebyshev polynomials are of both discrete and integral kinds, just as for their cousins the cosines that are used in Fourier expansions. Explicitly,

$$\sum_{i=1}^{n} T_l(x_{0i})T_m(x_{0i})=n\,\delta_{lm}(1+\delta_{m,0})/2, \quad l,m<n, \tag{8}$$

which is the analog of discrete Fourier transform orthogonality (for example, Ref. 10, Sec. 9.2), and

$$\int_{-1}^{1} \frac{T_l(x)T_m(x)}{\sqrt{1-x^2}}\,dx=\pi\delta_{lm}(1+\delta_{m,0})/2 \tag{9}$$

analogous to Fourier series orthogonality (Ref. 10, Sec. 9.4). The weight factor $1/\sqrt{1-x^2}$ accounts for the transformation between x and θ in Eq. (1). It does not give rise to any analytical singularities, but there may be numerical instabilities if an integrand of the form in Eq. (9) is evaluated directly for x near the end points.

Of the six classical orthogonal polynomials (Ref. 5, Sec. 3.4), the Chebyshev, Gegenbauer, and Jacobi polynomials are less familiar to physicists than are the other three—Hermite, Laguerre, and Legendre—presumably because the latter arise as solutions of Schrödinger equations for interesting potentials. Technically, the Chebyshev, Gegenbauer, and Legendre polynomials are special cases of Jacobi polynomials, but all six wise men of the 18th and 19th century are often acknowledged individually. Indeed, the procedures written in C that are in Baker's mathematical function handbook[11] compute T_n and U_n by using the recurrence relations for Jacobi polynomials given in Sec. 22.18 of Abramowitz and Stegun[9] rather than the defining Eqs. (1) and (2). Use of the Jacobi relations to compute T_n is not efficient.

Many other algebraic properties of Chebyshev polynomials are derived in Refs. 5, 8, and 12. We now discuss properties and algorithms that are particularly relevant and interesting for numerical applications. Fox and Parker's monograph[12] is a trove of information from the early days of computers, while Secs. 5.8–5.11 of *Numerical Recipes*[13] provide several practical algorithms and programs.

The minimax property

When approximating a given function $f(x)$ or a set of data in terms of fitting functions—usually because the latter is simpler to handle—one must specify what one means by a good approximation or "best fit." For example, there is the least-squares criterion, in which the sum of squares of deviations between given and fitting functions is minimized. An alternative criterion that is less familiar to physicists is the *minimax* best-fit criterion, in which one *mini*mizes the *max*imum absolute deviation between given and fitting functions over a certain interval. This may often be a more appropriate criterion than least squares, since it prevents wild oscillations of the fitting function about the data.

It is straightforward but lengthy to prove (Sec. 4.4 in Ref. 5, Chap. 2 in Ref. 8, Sec. 1.5 in Ref. 12) that the polynomial in x of nth degree that achieves the above minimax criterion is proportional to $T_n(x)$. Therefore, an expansion of the form

$$f(x)=\sum_{k=0}^{n-1} c_kT_k(x)+E_n(x) \tag{10}$$

will have minimal error (by the minimax criterion) for given n, with the error $E_n(x)$ being approximately proportional to $T_n(x)$. A practical application of this minimax property of Chebyshev polynomials is the radio-engineering problem of equalizing the sidelobes and obtaining the narrowest possible beam for n antennas that are equally spaced along a line with signals being fed in phase. The design of such an array, the Dolph–Chebyshev array, is discussed in Sec. 4.7 of Beckmann[5] and in Sec. 6.6 of Steinberg's monograph on aperture and array system design.[14] An extensive technical discussion of extremal properties of Chebyshev polynomials is given in Chap. 2 of Rivlin's monograph.[8]

Curve fitting and interpolation

A common use of orthogonal polynomials that satisfy discrete orthogonality relations such as Eq. (8) is to approximate a function $f(x)$ by a finite sum over n of the polynomials. For Chebyshev polynomials, we write

$$f(x)=\sum_{k=0}^{n-1} c_kT_k(x)+R_n(x), \tag{11}$$

which is a form that will look familiar to those who fit angular-distribution data, if T_k is replaced by the Legendre polynomial P_k and if $x=\cos\theta$. The term $R_n(x)$ is the error in approximating $f(x)$ by the finite sum; the smaller R_n is for convenient values of n and a chosen x, the better is the fit at x. From Eq. (8), we have the expansion coefficients c_k given by

$$c_k=2\sum_{i=1}^{n} f(x_{0i})T_k(x_{0i})/[n(1+\delta_{k,0})]. \tag{12}$$

In order to use this expression, the function f (which may be data) must be available at the roots x_{0i} given by Eq. (7). These are equally spaced in angle, but the angle steps depend upon the choice of n. This is an inconvenience that the Chebyshev expansion Eq. (11) has in common with the discrete Fourier transform using cosines or complex exponentials as the fitting functions. The parallel between Fourier and Chebyshev series is developed in Chap. 2 of Fox and Parker.[12] Note that in pure mathematics, "Fourier series" usually refers to an expansion in terms of *any* orthogonal functions, a fact that you may discover to your dismay if you peruse the math section in your science library.

It is straightforward to write a procedure in C (or a subroutine in Fortran) to evaluate the coefficients, or to borrow the recipe **chebft** from Press *et al.*[13] The c_k can then be used directly in Eq. (11) to interpolate estimates of $f(x)$, with the T_k being generated from Eq. (1). An alternative algorithm—Clenshaw's recurrence formula[15]—is sometimes more efficient. As applied to the T_k expansion, it is developed by noting that T_k satisfies the linear expansion relation Eq. (4). By using this recurrence in Eq. (11) and rearranging the summations, one can derive a recurrence relation for the coefficients c_k. The details and a procedure, **chebev**, are given in Secs. 5.5 and 5.8 of *Numerical Recipes.*[13] Its authors caution that, depending upon the direction of iteration (k increasing or decreasing), significant digits can be lost in the recurrence. A practical application of Chebyshev fitting and interpolation is described by Karas *et al.*[1]

Economizing series by Chebyshev approximations

Suppose that we have an approximation to e^x in terms of its Maclaurin series:

$$e^x = \sum_{i=0}^{n} \frac{x^i}{i!} + \frac{x^{n+1}}{(n+1)!} e^{\xi}, \quad |\xi| \leq 1. \tag{13}$$

If for simplicity we choose $n=6$, then for $x=1$, say, the error in truncating the expansion is about 2.0×10^{-4}, which is 0.3%. For $n=5$ and $x=1$, the error is 1.4×10^{-3}. If, however, we expand the same sum into Chebyshev polynomials, we obtain by using Eq. (5) for each power of x the result

$$\begin{aligned}\sum_{i=0}^{6} \frac{x^i}{i!} &= 1.26606T_0(x)+1.13021T_1(x)\\ &\quad +0.27148T_2(x)+0.04427T_3(x)\\ &\quad +0.00547T_4(x)+0.00052T_5(x)\\ &\quad +0.00004T_6(x)\end{aligned} \tag{14}$$

with the coefficients rounded to five decimals for simplicity. Since each T_k does not exceed unity, we can truncate the expansion after T_5 and the error is less than about 4×10^{-5}. This procedure of expanding a series into Chebyshev polynomials that is shorter than the original series for the same accuracy was named "economization" by Lanczos,[16] who developed the technique extensively.

It may seem tedious to calculate the coefficients in the Chebyshev expansion, as in Eq. (14). The procedure may, however, be automated in a function, for example **pccheb** in Sec. 5.11 of *Numerical Recipes.*[13] Whether economization produces a program that executes faster depends upon how quickly $T_k(x)=\cos(k \arccos x)$ can be computed compared to x^k. Alternatively, given an expansion such as Eq. (14), one can convert this into a power series with the same number of terms but with different coefficients than the original power series.

Rather than a power-series expansion of a function, such as Eq. (13), one can make an expansion into Chebyshev polynomials directly, with the coefficients in the expansion computed by using the integral orthogonality relation Eq. (9), as in Fourier expansions. For example (Sec. 4.5 in Fox and Parker[12]), keeping six decimals, we have

$$\begin{aligned}e^x &\approx 1.266066T_0(x)+1.130318T_1(x)\\ &\quad +0.271495T_2(x)+0.044337T_3(x)\\ &\quad +0.005474T_4(x)+0.000543T_5(x)\\ &\quad +0.000045T_6(x)\end{aligned} \tag{15}$$

in which the first four digits of each coefficient agree with those in Eq. (14). You can see immediately that you get five-decimal accuracy by keeping only seven terms. Many of our readers must have itchy fingers, wanting to type some of these formulas into the computer, and so in Box 2 we have a simple program that you can adapt to most programming languages and can modify to explore how the accuracy of the Chebyshev and series expansions depend on x. A sample comparison is shown in Fig. 2 for 7 terms in the expansions Eqs. (15) and (13). Notice the minimax property of the Chebyshev expansion—that the error oscillates about zero, rather than inexorably increasing as x increases, as it does for the power series.

Box 2. MATHEMATICA program for the Chebyshev approximation to seven terms of the exponential e^x, as given by Eq. (15). The error in the approximation is computed. In Fig. 2, it is compared to the error in the power-series expansion.

```
T[k_,x_] := Cos[k*ArcCos[x]]
ChebySum[x_] :=
   1.266066*T[0,x]+1.130318*T[1,x]+
   0.271495*T[2,x]+0.044337*T[3,x]+
   0.005474*T[4,x]+0.000543*T[5,x]+
   0.000045*T[6,x]
PowerSum[x_] := Sum[x^i/i!,{i,0,6}]

ChebyErr = Plot[Exp[x]-ChebySum[x],{x,-1,1},
           DisplayFunction->Identity];
PowerErr = Plot[Exp[x]-PowerSum[x],{x,-1,1},
           PlotStyle->{Dashing[{0.05}]},
           DisplayFunction->Identity];
Show[ChebyErr,PowerErr,
     DisplayFunction->$DisplayFunction];
```

Rivlin[8] provides (Chap. 3) an extensive treatment of the analysis of function expansions in series of Chebyshev polynomials, along with many algebraic examples. Rational functions in which the function is the quotient of two polynomials (Padé approximants) can also be approximated by Chebyshev polynomials. Examples are provided in Fox and Parker[12] Secs. 4.20–4.23. By using an adaptation of the Remez (or Remes) algorithms, Press *et al.*[13] (Sec. 5.13) give an algorithm and numerical program, while Release 2 of MAPLE V (Ref. 6) provides the numerical approximation package **numapprox** with five functions to automate constructing algebraic Chebyshev polynomial approximations of functions.

Numerical differentiation and integration

Suppose that we have the Chebyshev expansion as in Eq. (11), approximating a function f, so that

$$f(x) \approx \sum_{k=0}^{n-1} c_k T_k(x). \tag{16}$$

Approximate derivatives and integrals of f can be obtained in terms of those of the T_k. For example, the first derivative of f can be estimated from

$$f'(x) \approx \sum_{k=0}^{n-1} c_k' T_k(x) \tag{17}$$

in which the coefficients for the derivative expansion, the c_k', can be derived in terms of the c_k by differentiating both sides in the top formula in Eq. (4) then writing out Eq. (17) in terms of contiguous T_k. The recurrence relation between the derivative coefficients is thus

$$c_{k-1}' = c_{k+1}' + 2(k-1)c_k, \quad k=n-1,n-2,\ldots,2, \tag{18}$$

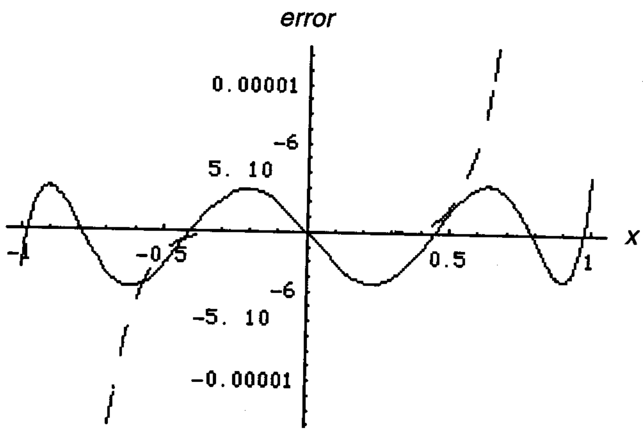


Figure 2. Error in the Chebyshev expansion Eq. (15) to seven terms shown as the solid curve and in the power-series expansion Eq. (13) to seven terms shown as the dashed curve for $|x|<0.7$. Prepared using the program in Box 2.

$$c'_n = c'_{n-1} = c'_0$$

in which the first two zero conditions arise from our ignorance of the higher-order coefficients in expansion (16) for f. This algorithm is implemented in, for example, procedure **chder** described in Sec. 5.9 of *Numerical Recipes.*[13] From this introductory discussion, it is clear that solving differential equations can also be helped by using Chebyshev polynomials. Several methods are under extensive development by mathematicians, for example in Ref. 17, and a practical implementation in hydrodynamics is described by Shen.[4]

Chebyshev polynomials can also be rushed into help with integration. The simplest method is to begin with approximation (16) and to write the indefinite integral of f in terms of those of the T_k. The integral relation

$$\int T_k(x)dx = \frac{1}{2}\left(\frac{1}{k+1}\,T_{k+1}(x) - \frac{1}{k-1}\,T_{k-1}(x)\right), \quad k>1,$$

$$\int T_0(x)dx = T_1(x), \tag{19}$$

$$\int T_1(x)dx = 1/4[T_0(x)+T_2(x)]$$

follows from the definition Eq. (1) and integrals of trigonometric functions. It can be used to approximate the integral of f as

$$\int f(x)dx \approx \sum_{k=0}^{n} C_k T_k(x) \tag{20}$$

in terms of the coefficients C_k that satisfy the recurrence relation

$$C_k = \frac{c_{k-1} - c_{k+1}}{2(k-1)}, \quad k>1, \quad C_1 = c_1. \tag{21}$$

The choice of C_0 is arbitrary, since there is an arbitrary constant of integration. This integration algorithm is implemented in the *Numerical Recipes* procedure **chint**. The work of Yahiro and Gondo[2] on two-electron Gaussian integrals provides a practical example of using Chebyshev approximations for integration.

A constant challenge to those who devise numerical algorithms is to devise schemes that perform integrals reliably, efficiently, and to specified accuracy for a wide range of functions. Pérez-Jordá, San-Fabián, and Moscardó have recently provided a modified Gauss–Chebyshev algorithm and a compact FORTRAN-77 program to perform automatic numerical integration.[18]

Overall, as we see from this introduction to their many practical applications, after the spelling the rest is easy with Chebyshev polynomials.

Further reading

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In the next issue: Mathematica and Maple: Has Champaign met its Waterloo?