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Minimax approximations to the zeros of $P_n(x)$ and Gauss–Legendre quadrature

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Abstract

This paper is concerned with the numerical development of some minimax trigonometric approximations to the positive zeros of the nth Legendre polynomial $P_n(x)$. One of the approximation formulas we derive yields at least 4.2 significant decimal digits of accuracy for any $n \geqslant 2$, and can be used to furnish initial guesses in an iterative method for the computation of the zeros of $P_n(x)$ to nearly full machine accuracy. This approach avoids some of the computational complexity associated with the selection of appropriate initial guesses for use in a special 5th order scheme previously developed by the first author for the numerical computation of the abscissas required in the n-point Gauss–Legendre quadrature rule.

Keywords: Legendre polynomials; Asymptotic approximation; Gauss–Legendre quadrature

1. Introduction

In the following work it is convenient to let $x_{n,k}$, $k = 1, 2, \ldots, n$ denote the zeros of the nth Legendre polynomial $P_n(x)$, normalized by the condition $P_n(1) = 1$. To save a multiplication $P_n(x)$ can be computed in a stable manner from the classical three-term recurrence relation rewritten in the form [6]:

$$P_n(x) = \left(1 - \frac{1}{n}\right)[xP_{n-1}(x) - P_{n-2}(x)] + xP_{n-1}(x), \quad n \geqslant 2,$$

where $P_0(x) = 1$, $P_1(x) = x$. It is well known [10] that the n zeros of $P_n(x)$ are real, distinct and in the open interval $(-1, 1)$, and we employ the labeling convention

$$-1 < x_{n,n} < \cdots < x_{n,2} < x_{n,1} < 1.$$

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Furthermore, the $x_{n,k}$ satisfy the symmetry property

$$x_{n,k} = -x_{n,n+1-k}, \quad k = 1,2,\ldots,[\tfrac{1}{2}n],$$

where $[\frac{1}{2}n]$ denotes the integer part of $\frac{1}{2}n$, and for odd n we have $x_{n,[\frac{1}{2}n]+1} = 0$. Consequently, attention can be restricted to the $[\frac{1}{2}n]$ positive zeros

$$0 < x_{n,[\frac{1}{2}n]} < \cdots < x_{n,2} < x_{n,1} < 1.$$

These zeros are important because they are the abscissas in the n-point Gauss–Legendre quadrature rule,

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \delta_n w_{n,[\frac{1}{2}n]+1} f(0) + \sum_{k=1}^{[\frac{1}{2}n]} w_{n,k}[f(x_{n,k}) + f(-x_{n,k})],$$

where $\delta_n = 1$ if n is odd, $\delta_n = 0$ if n is even, and

$$w_{n,k} = 2 \Big/ \sum_{k=0}^{n-1} (2k+1)[P_k(x_{n,k})]^2.$$

For $n \to \infty$, asymptotic approximations to the zeros $x_{n,k}$ can be found in the literature on orthogonal polynomials and the special functions [3, 8, 10]. These asymptotic approximations are generally of two types. The first type involves the kth positive root j_k of the Bessel function $J_0(x)$, as illustrated by Gatteschi's [3, 4] asymptotic approximation

$$x_{n,k} = \cos\left\{\frac{j_k}{\sqrt{n^2+n+\frac{1}{3}}}\left(1 - \frac{j_k^2 - 2}{360(n^2+n+\frac{1}{3})^2}\right)\right\} + \mathrm{O}(n^{-7}). \tag{1.1}$$

The second type involves trigonometric functions, as depicted by Tricomi's [11, 12] asymptotic approximations

$$x_{n,k} = \{1 - \tfrac{1}{8}n^{-2} + \tfrac{1}{8}n^{-3} - \tfrac{1}{384}n^{-4}(39 - 28\csc^2\theta_{n,k})\}\cos\theta_{n,k} + \mathrm{O}(n^{-5}) \tag{1.2}$$

and

$$x_{n,k} = (1 - \tfrac{1}{8}n^{-2} + \tfrac{1}{8}n^{-3})\cos\theta_{n,k} + \mathrm{O}(n^{-4}), \tag{1.3}$$

where

$$\theta_{n,k} = \frac{k - \frac{1}{4}}{n + \frac{1}{2}}\pi. \tag{1.4}$$

Numerical experiments [7] show that for a fixed value of n, the accuracy of each of these asymptotic approximations varies widely depending on the value of k in the allowable range $1 \leqslant k \leqslant [\frac{1}{2}n]$. Asymptotic approximations such as (1.1) are generally the most accurate for approximating the largest zeros near $+1$, whereas trigonometric approximations such as (1.2) and (1.3), respectively, provide better approximations for the middle and smaller positive zeros of $P_n(x)$. This is the reason for the method suggested in Ref. [7] for obtaining initial approximations to $x_{n,k}$: use (1.1) if $k = 1$, (1.2) if $2 \leqslant k \leqslant [\frac{1}{3}n]$, and (1.3) if $[\frac{1}{3}n] < k \leqslant [\frac{1}{2}n]$. The latter hybrid scheme was used in Ref. [7] to supply initial guesses for a special 5th order iterative method in order to compute, with a single iteration, all the positive zeros of $P_n(x)$ correct to at least 20 significant decimal digits.

The main purpose of this paper is to use numerical optimization techniques to develop some minimax trigonometric approximations to $x_{n,k}$ that are more uniformly accurate, for all $n \geqslant 2$ and $1 \leqslant k \leqslant [\frac{1}{2}n]$, than their classical asymptotic counterparts. Of these we mention the convenient near minimax approximation

$$x_{n,k} \approx \Omega_{n,k} = [1 - \tfrac{1}{8}n^{-2} + \tfrac{5}{38}n^{-3} - \tfrac{2}{25}n^{-4}(1 - \tfrac{14}{39}\theta_{n,k}^{-2})] \cos \theta_{n,k}. \tag{1.5}$$

It will be shown that unlike the motivating classical approximation (1.2), the approximation (1.5) can be used to compute $x_{n,k}$ correct to at least 4.2 significant decimal digits of accuracy for any $n \geqslant 2$ and $1 \leqslant k \leqslant [\frac{1}{2}n]$.

For any $n \geqslant 2$, the near minimax approximation (1.5) can be used as an initial guess with one iteration of the special 5th order scheme given in Ref. [7],

$$x_{n,k} \approx E_5^*(\Omega_{n,k}) \tag{1.6}$$

to compute $x_{n,k}$ to nearly full IEEE double precision accuracy. For completeness and to correct a typographical error in Ref. [7], we record

$$E_5^*(x) = x - (1 - x)(1 + x)v(1 + v(x + v(B + Cv))),$$

where

$$v = \frac{P_n(x)}{n[P_{n-1}(x) - xP_n(x)]},$$

$$B = \tfrac{1}{3}(3 + n(n + 1))x^2 - \tfrac{1}{3}(1 + n(n + 1))$$

and the corrected coefficient

$$C = \tfrac{1}{6}(6 + 5n(n + 1))x^3 - \tfrac{1}{6}(4 + 5n(n + 1))x.$$

2. Minimax approximations to the positive zeros

It is useful for our purposes to arrange the positive zeros of the Legendre polynomials in the triangular scheme shown in Fig. 1, where the kth positive zero $x_{n,k}$ of $P_n(x)$ is in row $n - 1$ and column k. For a given value of $N > 2$, introduce the set of indices

$$I_N = \{(n, k) \colon 2 \leqslant n \leqslant N,\ 1 \leqslant k \leqslant [\tfrac{1}{2}n]\}$$

corresponding to the zeros in the upper, finite triangular portion of Fig. 1, and let

$$I_\infty = \{(n, k) \colon 2 \leqslant n < \infty,\ 1 \leqslant k \leqslant [\tfrac{1}{2}n]\}.$$

For a given m-parameter model $M_{n,k}(\boldsymbol{p})$, we wish to develop approximations of the form $x_{n,k} \approx M_{n,k}(\boldsymbol{p})$, $(n, k) \in I_\infty$, where the choice of the m coefficients in the parameter vector $\boldsymbol{p} = (p_1, p_2, \ldots, p_m)$ remains at our disposal in order to minimize the maximum relative error associated with the latter approximation.

$$
\begin{array}{llll}
x_{2,1} & & & \\
x_{3,1} & & & \\
x_{4,1} & x_{4,2} & & \\
x_{5,1} & x_{5,2} & & \\
\bullet & \bullet & & \\
x_{N,1} & x_{N,2} & \bullet\bullet\bullet & x_{N,[N/2]} \\
\bullet & \bullet & & \bullet
\end{array}
$$

Fig. 1. Triangular scheme for positive zeros $x_{n,k}$, $n \geqslant 2$, $1 \leqslant k \leqslant [\frac{1}{2}n]$.

As illustrated in the examples below, viable candidates for the m-parameter model $M_{n,k}(\boldsymbol{p})$ can be obtained by modifying some of the known asymptotic approximations formulas for $x_{n,k}$. The basic idea is to first choose the form of the model $M_{n,k}(\boldsymbol{p})$ so that the model accurately mimics the behavior of a known asymptotic approximation for $(n, k) \in I_\infty \backslash I_N$, $N \gg 2$, and then use a numerical optimization method to calculate the vector $\boldsymbol{p} = \boldsymbol{q}$, that minimizes the maximum relative error

$$R_N(\boldsymbol{p}) = \max_{I_N} |r_{n,k}(\boldsymbol{p})|, \tag{2.1}$$

where

$$r_{n,k}(\boldsymbol{p}) = \frac{x_{n,k} - M_{n,k}(\boldsymbol{p})}{x_{n,k}}.$$

If N is sufficiently large we would expect $M_{n,k}(\boldsymbol{q})$ to approximate accurately not only the zeros $x_{n,k}$ in the upper, finite triangular part of Fig. 1 with $2 \leqslant n \leqslant N$, but also the zeros with indices $n > N$ in the lower, infinite part of Fig. 1. Under these conditions we obtain a minimax approximation

$$x_{n,k} \approx M_{n,k}(\boldsymbol{q}) \quad (n, k) \in I_\infty \tag{2.2}$$

for the positive zeros of the Legendre polynomials. The number of significant decimal digits of accuracy afforded by the approximation (2.2) is given by

$$d_{n,k}(\boldsymbol{q}) = -\log_{10} |r_{n,k}(\boldsymbol{q})| - \log_{10} 2.$$

In this latter regard it is helpful to determine numerically the least number of significant decimal digits of accuracy

$$\mu(\boldsymbol{q}) = \operatorname*{Infimum}_{I_\infty} |d_{n,k}(\boldsymbol{q})|$$

attained by (2.2), which we would expect to be given by

$$\mu(\boldsymbol{q}) = -\log_{10} R_N(\boldsymbol{q}) - \log_{10} 2.$$

In practice, a suitable value of N for use in (2.1) must be determined experimentally. For the models we considered, $N = 20$ was adequate. If the number of free parameters m is not too large, the simplex algorithm of Nelder and Mead [1] can be used to minimize $R_{20}(\boldsymbol{p})$, and thereby calculate $\boldsymbol{q}$ in order to obtain the desired minimax approximation (2.2). Among the several models we investigated, the following two examples serve to illustrate the general type of result that can be obtained using the above approach.

Example 1. The classical asymptotic approximation [3, Eq. (7.14.12)]

$$x_{n,k} = \frac{n^2 + 2n + \frac{5}{8}}{n^2 + 2n + \frac{3}{4}} \cos\theta_{n,k} + \mathrm{O}(n^{-2}) \tag{2.3}$$

suggests the two-parameter model

$$M_{n,k}(p_1, p_2) = \frac{n^2 + 2n + p_1}{n^2 + 2n + p_2} \cos\theta_{n,k}, \tag{2.4}$$

where, as before, $\theta_{n,k}$ is defined by (1.4). For the two-parameter model (2.4), $R_{20}(\boldsymbol{p})$ is minimized when $\boldsymbol{p} = \boldsymbol{q} = (-0.478683, -0.341487)$, the corresponding minimax approximation, $M_{n,k}(\boldsymbol{q})$, giving $R_{20}(\boldsymbol{q}) = 0.00016$ and $\mu(\boldsymbol{q}) = 3.5$. In contrast to the latter minimax approximation, the classical approximation furnished by (2.3) is $M_{n,k}(\boldsymbol{s})$, where $\boldsymbol{s} = (\frac{5}{8}, \frac{3}{4})$, and we find $R_{20}(\boldsymbol{s}) = 0.0035$ and $\mu(\boldsymbol{s}) = 2.2$. For each $k = 1, 2, \ldots, 50$ and $n = 2, \ldots, 100$, we plot in Fig. 2 the significant digits of accuracy $d_{n,k}(\boldsymbol{q})$ and $d_{n,k}(\boldsymbol{s})$, afforded by the respective minimax approximation $M_{n,k}(\boldsymbol{q})$ and the classical approximation $M_{n,k}(\boldsymbol{s})$. For purposes of clarity, only a few of the significant digits of accuracy curves are labeled with their corresponding values of k.

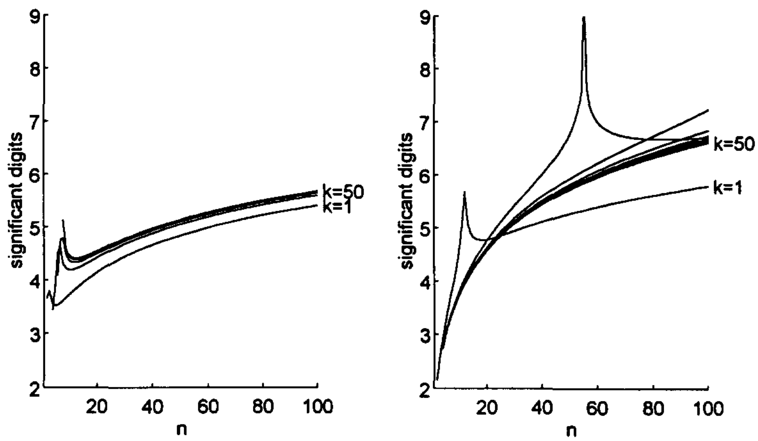

Fig. 2. Left: Significant digits $d_{n,k}$ for minimax model $M_{n,k}(\boldsymbol{q})$ in Example 1. Right: Significant digits $d_{n,k}$ for classical model $M_{n,k}(\boldsymbol{s})$ in Example 1.

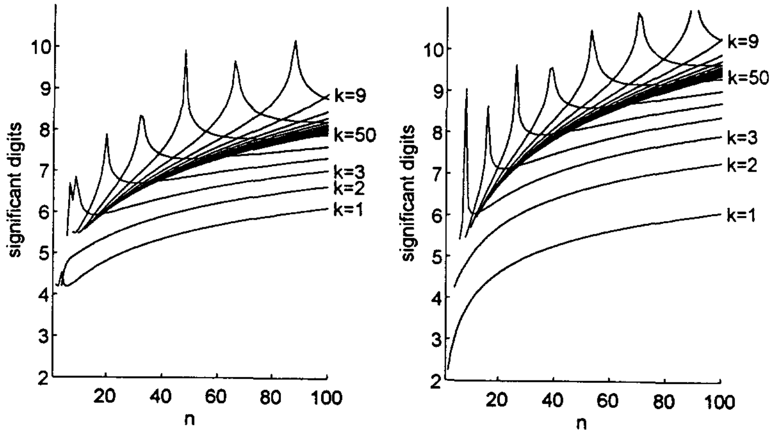

Fig. 3. Left: Significant digits $d_{n,k}$ for near minimax approximation (1.5). Right: Significant digits $d_{n,k}$ for classical approximation (1.2).

Example 2. The classical asymptotic approximation (1.2) suggests the $m = 3$ parameter model

$$M_{n,k}(\boldsymbol{p}) = \left[1 - \frac{1}{8n^2} + \frac{p_1}{n^3} - \frac{p_2}{n^4}\left(1 - \frac{p_3}{\theta_{n,k}^2}\right)\right]\cos\theta_{n,k}. \tag{2.5}$$

For (2.5), $R_{20}(\boldsymbol{p})$ is minimized when $\boldsymbol{p} = \boldsymbol{q} = (0.131566, 0.080040, 0.359007)$. It is convenient to employ the simple approximation $\boldsymbol{q} \approx \boldsymbol{t} = (\frac{5}{38}, \frac{2}{25}, \frac{14}{39})$ and investigate the corresponding near minimax approximation $M_{n,k}(\boldsymbol{t}) = \Omega_{n,k}$, introduced previously by (1.5). For the approximation $M_{n,k}(\boldsymbol{t}) = \Omega_{n,k}$, we find $R_{20}(\boldsymbol{t}) = 0.0000325$ and $\mu(\boldsymbol{t}) = 4.2$. In contrast to the near minimax approximation (1.5), the classical approximation (1.2) has $R_{20} = 0.00279$ and $\mu = 2.3$. Finally, for each $k = 1, 2, \dots, 50$ and $n = 2, \dots, 100$, we plot in Fig. 3 the significant digits of accuracy attained by the near minimax approximation (1.5) and the corresponding classical approximation (1.2).

3. Minimax approximations for the largest zeros

It is interesting to develop some special minimax approximations for the largest zero $x_{n,1}$, $n \geqslant 2$. As might be expected, the resulting special approximations to $x_{n,1}$ offer greater accuracy than can be obtained by simply taking $k = 1$ in more general approximations to $x_{n,k}$.

The simple approximation $x_{n,1} \approx \cos\theta_{n,1}$ yields no more than 1.4 digits when $n = 2$ and slowly increases to 4.6 significant decimal digits when $n = 100$. The fact that $\theta_{n,1}$ is a proper rational function of n, with the degree of the numerator one less than the degree of the denominator suggests the family of $2i + 1$ parameter models

$$x_{n,1} \approx \cos\frac{a_1 n^i + a_2 n^{i-1} + \cdots + a_{i+1}}{b_1 n^{i+1} + b_2 n^i + \cdots + b_i n + 1}. \tag{3.1}$$

For a given value of the nonnegative integer i, we can determine numerically the $2i + 1$ a's and b's in (3.1) to minimize the relative error afforded by the approximation (3.1) for $n \geqslant 2$. The next two examples summarize the numerical results obtained for the cases $i = 0, 1$.

Example 3. For $i = 0$, the minimax approximation is

$$x_{n,1} \approx \cos \frac{a_1}{b_1 n + 1}$$

where $a_1 = 4.5779491$, $b_1 = 1.8958083$. This approximation yields at least 3.6 significant decimal digits of accuracy for all $n \geqslant 2$.

Example 4. For $i = 1$, the minimax approximation is

$$x_{n,1} \approx \cos \frac{a_1 n + a_2}{b_1 n^2 + b_2 n + 1},$$

where $a_1 = 13.1968145$, $a_2 = 3.78439578$, $b_1 = 5.48752506$, $b_2 = 4.31972733$. This approximation yields at least 6.8 significant decimal digits of accuracy for all $n \geqslant 2$.

Finally, we develop a minimax approximation in Example 5 that illustrates the substantial improvement in accuracy that can sometimes be realized by perturbing some of coefficients in a classical asymptotic approximation. In particular, for $k = 1$ the classical approximation furnished by (1.1) is

$$x_{n,1} \approx \cos \left\{ \frac{j_1}{\sqrt{n^2 + n + \frac{1}{3}}} \left(1 - \frac{j_1^2 - 2}{360(n^2 + n + \frac{1}{3})^2} \right) \right\}, \tag{3.2}$$

where $j_1 = 2.4048255577$ is the first positive zero of the Bessel function $J_0(x)$. The approximation (3.2) yields at least 4.4 significant decimal digits of accuracy for all $n \geqslant 2$. Replacing the two constants $j_1^2 - 2$ and $\frac{1}{3}$, in the rightmost part of the classical approximation (3.2), with the two free parameters a_1 and b_1 furnishes a model whose relative error can be minimized over all $n \geqslant 2$. This approach gives the following result.

Example 5. The minimax approximation

$$x_{n,1} \approx \cos \left\{ \frac{j_1}{\sqrt{n^2 + n + \frac{1}{3}}} \left(1 - \frac{a_1}{360(n^2 + n + b_1)^2} \right) \right\}$$

has coefficients $a_1 = 0.0105077313672$, $b_1 = 0.165291040565$, and yields at least 9.4 significant decimal digits of accuracy for all $n \geqslant 2$.

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