

A numerical computation of special functions with applications to physics

Kganya Motsepe^α, Igor Fedotov,
Michael Shatalov^β and Stephan V Joubert

Department of Mathematics and Statistics
Tshwane University of Technology
Pretoria, South Africa

Abstract

Students of mathematical physics, engineering, natural and biological sciences sometimes need to use special functions that are not found in ordinary mathematical software. In this paper a simple universal numerical algorithm is developed to compute the Legendre function values of the first kind using the Legendre differential equation. The computed function values are compared to built-in values in *Mathcad14* and *Derive6*. Error analysis is performed to test the accuracy of the algorithm. Graphical residuals are found to be of order 10^{-12} . Finally, some physical application is presented.

1 Introduction and motivation

Abramowitz and Stegun's Handbook of Mathematical Functions [1] is one of the most cited references in mathematics. According to Ludovic and Bruno [2] the formulas in this book on special functions were computed, written and proof-read by hand.

The method of separation of variables for the solution of partial differential equations often leads to ordinary differential equations (ODEs) with variable coefficients. The solutions are obtained in the form of infinite series or in terms of special functions. The Legendre and Bessel equations are some of the ordinary differential equations derived from the wave equation. These equations and their solutions play an important role in applied mathematics, electric field, heat conduction, fluid flow *et cetera* (see for example, Lebedev [9], Tikhonov and Samarskii [3]).

The main objective of this paper is to develop a simple numerical method using the Legendre differential equation:

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + n(n+1)y = 0 \quad (0.1)$$

which could be re-written as:

^α motsepeka@tut.ac.za

^β Permanent address: Sensor Science and Technology of CSIR Manufacturing and Materials, P.O. Box 305, Pretoria 0001, South Africa

$$\frac{d^2 y}{dx^2} - \frac{2x}{(1-x^2)} \frac{dy}{dx} + \frac{n(n+1)}{(1-x^2)} y = 0 \quad (0.2)$$

with given initial values to compute numerical values of the Legendre polynomials. The computed function values will be compared carefully against built-in values in *Mathcad14* and *Derive6* software. As an application in physics, the concept of sound scattering by a sphere will be presented.

2 The algorithm

At present there are a wide variety of computer packages that include differential equation solvers. In general these packages contain all of the input/output and integration algorithms and the user, only has to specify the equation to solve. In this paper the *Mathcad14* and the *Derive6* package will be used as a differential equation solver with their respective functions which are called are Rkadapt [4] and RK [5] and [6]. The two functions are the Runga-Kutta methods of order four.

The first step in solving a second order initial value problem is to recast the second order equation into two simultaneous first order differential equations. From (0.2), let

$$\begin{aligned} \frac{dy}{dx} &= z \\ \frac{dz}{dx} &= \frac{2x}{1-x^2} z - \frac{n(n+1)}{1-x^2} y. \end{aligned} \quad (2.1)$$

The derivatives $\frac{dy}{dx}$ and $\frac{dz}{dx}$ are written as functions of x , y and z . Using *Mathcad* the two equations in (2.1) are put into a “ D ” format by defining $D(x, y)$ as a 2×1 column vector, with $\frac{dy}{dx}$ as the first element and $\frac{dz}{dx}$ as the second element [5]. Next the initial conditions for both y and $\frac{dy}{dx}$ are set and are also written as a 2×1 column vector.

```

n := 10

ye := (1
      0)

De(x, ye) := [
              ye_1
              (1-x)^2
              ye_1 - n*(n+1) * (ye_0 / (1-x)^2)
            ]

Ye := Rkadapt (ye, 0, 0.999, 1000, De)
    
```

Figure 1: Mathcad syntax for $P_{10}(x)$

The next step is to solve the System (2.1) by invoking the Runge-Kutta solver by using the Rkadapt function. The output is a three-column matrix in which the first column contains the independent variable x , the second column contains the solutions for the dependent variable y and the third column represents the second dependent variable $\frac{dz}{dx}$. Each successive row is a solution for that respective time-step.

The command needed to start the integration has the form: $Rkadapt(y_e, x_1, x_2, N, D)^4$, where y_e is a vector of initial values and x_1 and x_2 are the end points of the integration interval. N is the number of points (in addition to the initial value) which need to be calculated and D is a vector that defines how the first order derivatives are evaluated. An example will best describe how to use this function.

The example of a Legendre polynomial of degree ten, $P_{10}(x)$ will be computed with initial values (1,0) and the corresponding Mathcad syntax is shown below in Figure 1 above, where z is represented by ye_1 and y is represented by ye_0 . The subscript, “e”, signifies that the function is an even function. The Derive syntax is shown in Figure 2.

```

EXTRACT_2_COLUMNS ( RK ( [ z, (2*x*z) / (1-x)^2 - (n*(n+1)*y) / (1-x)^2 ], [x, y, z], [0, -0.24609375, 0],
0.000999, 15 ], 1, 2 )
    
```

Figure 2: Derive syntax for $P_{10}(x)$

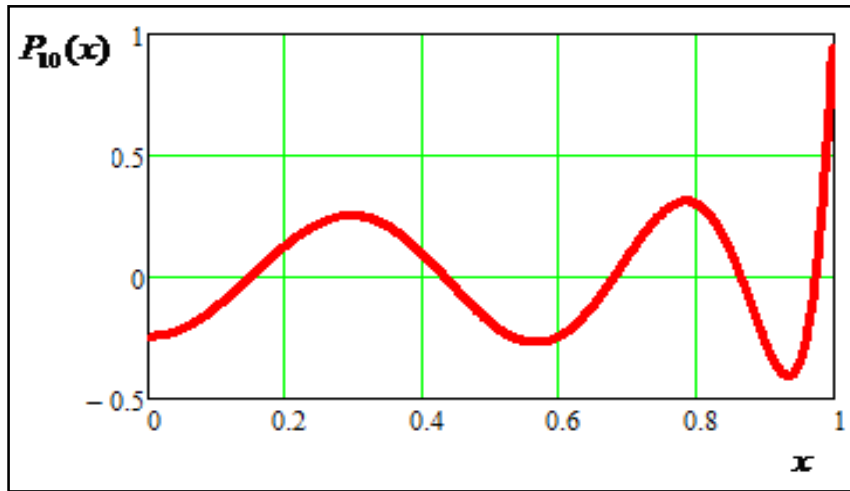


Figure 3: Graph of Legendre Polynomial $P_{10}(x)$ using Mathcad

The graphical solution is shown in Figure 3 and the corresponding function values are shown in Table 1.

Table 1: Numerical Legendre polynomial values for $P_{10}(x)$

MATHCAD		DERIVE	
x	$P_{10}(x)$		
0	-0.24609375	0	-0.24609375
0.000999	-0.24608024	0.000999	-0.24608024
0.001998	-0.24603972	0.001998	-0.24603971
0.002997	-0.24597219	0.002997	-0.24597218
0.003996	-0.24587765	0.003996	-0.24587765
0.004995	-0.24575612	0.004995	-0.24575612
0.005994	-0.24560761	0.005994	-0.2456076
0.006993	-0.24543213	0.006993	-0.24543213
0.007992	-0.24522971	0.007992	-0.24522971
0.008991	-0.24500036	0.008991	-0.24500036
0.009990	-0.24474411	0.00999	-0.2447441
0.010989	-0.24446098	0.010989	-0.24446098
0.011988	-0.24415101	0.011988	-0.244151
0.012987	-0.24381422	0.012987	-0.24381421
0.013986	-0.24345065	0.013986	-0.24345064
0.014985	-0.24306034	0.014985	-0.24306033

The values shown here are only in the interval from $x = 0$ to $x = 0.014985$, taking the step size of $h = 0.000999$, that is, a very small interval. The corresponding polynomial values can also be computed in *Derive6* using the Runge-Kutta method of order four. The function to call the algorithm is $RK(r, v, v_0, h, n)$ (see [5] and [6]), which approximates the solution of the first order differential equations (2.1). The symbol r represents a vector of expressions on the right hand side of (2.1), v is a three column vector of the unknowns x, y and z , h is the desired step size and n is the desired number of steps.

Visual inspection of table 1 shows the two numerical solutions are more or less the same except some slight differences at randomly placed step sizes and the

difference is seen in the eighth decimal digit. In section 3 the accuracy of the algorithm is investigated.

3 Accuracy of the Algorithm

Joubert and Greeff [7] developed a method for checking the accuracy of the numerical solutions of higher order ordinary differential equations. According to their method the Legendre differential equation (0.1) is differentiated once to obtain the third order differential equation

$$(1-x^2)\frac{d^3y}{dx^3} - 4x\frac{d^2y}{dx^2} + [n(n+1) - 2]\frac{dy}{dx} = 0. \tag{3.1}$$

Equation (3.1) is transformed into a 3 x 3 system of first order equations, which are

$$\begin{aligned} \frac{dy}{dx} &= y_1 \\ \frac{dy_1}{dx} &= y_2 \\ \frac{d^2y_1}{dx^2} &= \frac{4x}{1-x^2}y_2 + \frac{[2-n(n+1)]}{1-x^2}y_1. \end{aligned} \tag{3.2}$$

The next step is to solve the System (3.2) together with the given initial values to obtain its numerical solution. To check for the accuracy of the algorithm, the graphical solutions of Systems (2.1) and (3.2) are visually compared. The syntax for Systems (2.1) and (3.2) are shown together in Figure 4.

```

n := 10          TOL := 10-8
ye := (1)
           (0)
yz := ( 1 )
           0
          (-n2 - n)
De(x, ye) := [ ye1
               (2x / (1-x2)) * ye1 - n * (n+1) * (ye0 / (1-x2)) ]
Dz(x, yz) := [ yz1
               yz2
               (4x / (1-x2)) * yz2 + ((2-n2-n) / (1-x2)) * yz1 ]
Ye := Rkadapt(ye, 0, 0.999, 1000, De)
N := last(Ye<0>)    i := 0..N    N = 1000    Yz := Rkadapt(yz, 0, 0.999, 1000, Dz)
    
```

Figure 4: Mathcad syntax for Systems (2.1) and (3.2) for $P_{10}(x)$

The graphical solutions of the two systems are depicted in Figure 5.

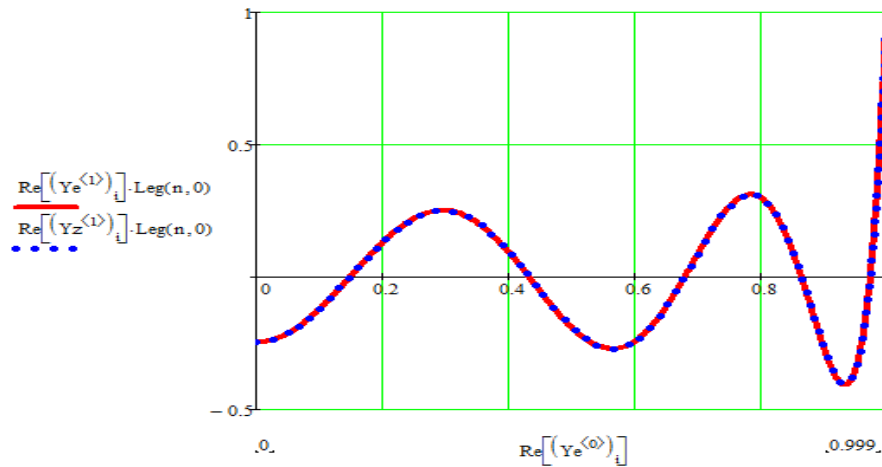


Figure 5: Graphs of the solutions to Systems (2.1) and (3.2) for $P_{10}(x)$

Visually the two graphical numerical solutions coincide. To support the visual check one can construct the graph of the absolute estimated error between the two numerical solutions of Systems (2.1) and (3.2). The graph of absolute estimated error is shown in Figure 6 and it can be seen that the absolute estimated error is less than 10^{-10} . Hence the Joubert-Greeff test [7] for accuracy indicates that the solution is accurate to at least 8 significant figures over the interval $[0,0.999]$.

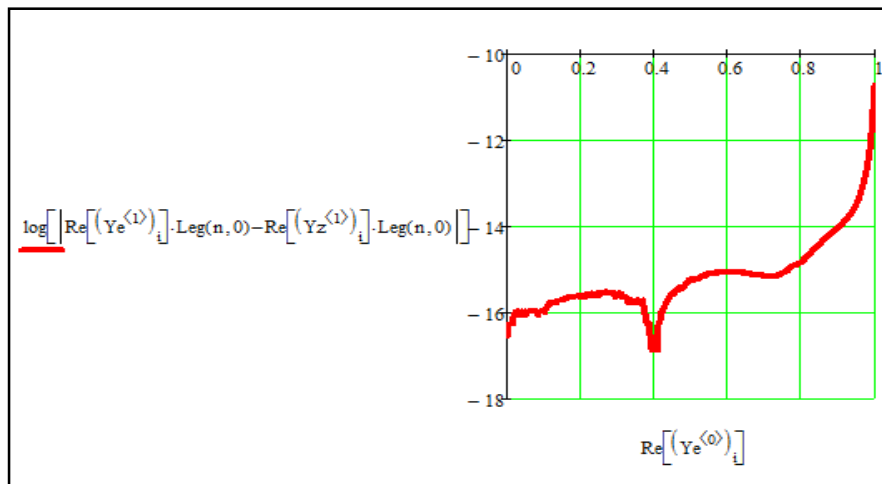


Figure 6: Graph of absolute estimated error for $P_{10}(x)$

4 Application to acoustics

In this section the scattering of sound by a solid sphere is considered. Consider a distance point sound source, which generates a continuous sound wave. At points, which are far away from this source and over suitably restricted regions, these waves may be said to approximate plane waves [8] see Figure 7.

A plane sound wave, propagating in the direction of the x-axis, that is, in the direction of $\theta = 180^\circ$, is incident, on a perfectly rigid and stationary sphere of radius R . The centre of the sphere is at the origin of the rectangular coordinates. See Figure 7 for the scattered pressure wave.

According to Jacobson and Juhl¹⁰ the numerical formula for the scattered sound pressure is defined as:

$$p(\theta, r, N) = \sum_{m=0}^N \left[(2m+1) \cdot i^{-m} \cdot \frac{dj(m, kR)}{dh(m, kR)} \cdot h(m, kR) \cdot Leg(m, \cos \theta) \right] \quad (4.1)$$

Formula (4.1) can be programmed in *Mathcad*, where $dj(m, kR)$ represents the derivative of the numerical spherical Bessel functions of the first kind with fractional order and $dh(m, kR)$ are the derivatives of the spherical Hankel functions and N represents the number of terms that can be summed. The sound pressure is a complex quantity and it is therefore practical to convert it to a quantity that can be easily graphed. This interesting quantity is sound intensity,

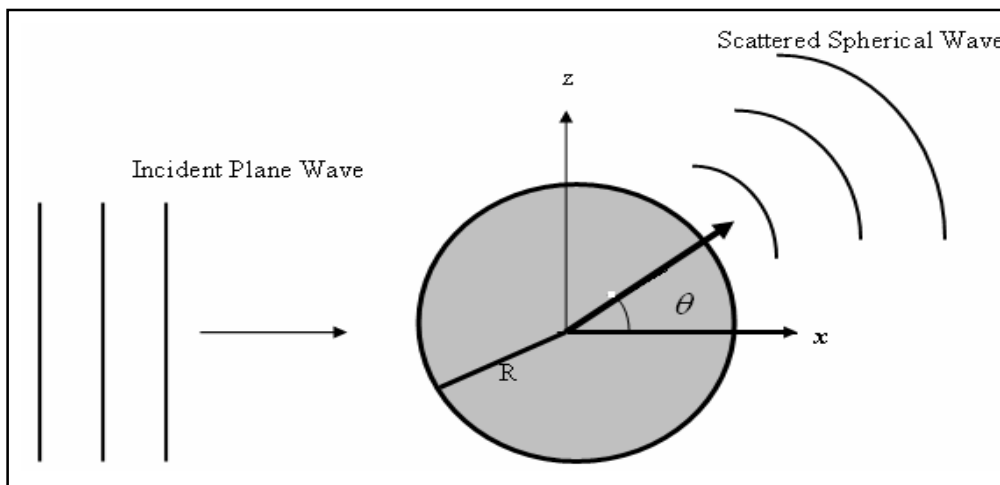


Figure 7: Geometrical diagram for sound scattering from a rigid sphere

which according to Tikhonov and Samarskii [3] and Jacobson and Juhl [10] can be defined as the square of sound pressure. Thus, to compute sound intensity one needs to multiply sound pressure by its complex conjugate. Therefore sound intensity is defined as

$$I(\theta, r, N) = p(\theta, r, N) \times \overline{p(\theta, r, N)}. \quad (4.2)$$

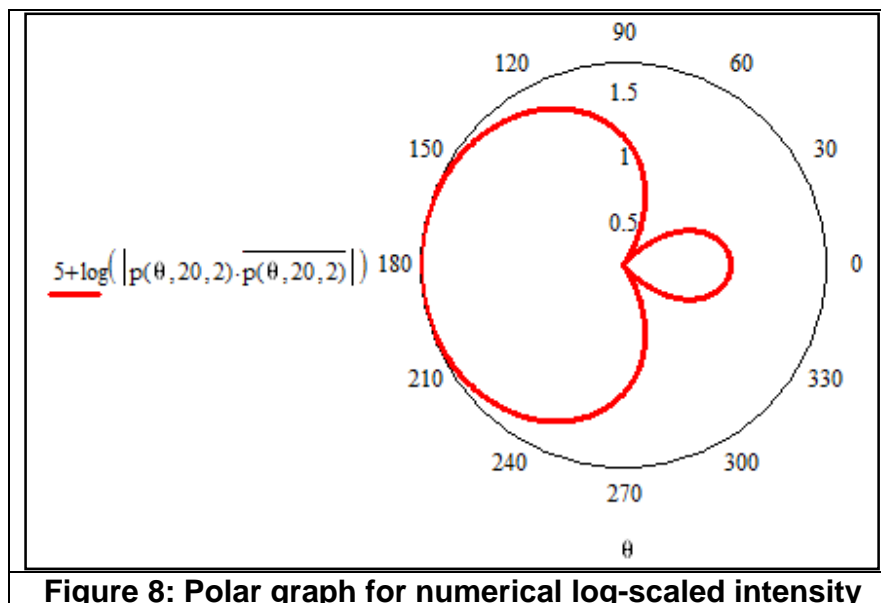
The sound intensity is dependent on the direction angle θ and the distance r from the sphere. The polar diagram for the numerical intensity of the sound scattered from a sphere is shown in Figure 8.

As can be seen the sound intensity is drawn using the decimal logarithmic scale and this is due to the very small numbers or very large numbers that are encountered in the study of sound. The very small or large numbers are easily reduced to manipulative numbers by introducing the decimal logarithm scale.

When observing the polar graph one notices that in front of the scatterer there is a big lobe, which shows that the intensity of the scattered sound is high on the frontal position. Behind the sphere the lobe is small, confirming that the sound intensity is lower on the leaside.

This phenomenon can be observed in built-up areas where high walls are constructed to bar the noise of the passing traffic, which is a disturbance to residents.

From this section, which involved application to acoustics, it can be observed that Legendre polynomials play an important role in the study of acoustics, since they determine the directivity properties of the scattered sound wave.



5 Concluding remarks

In this paper a numerical method algorithm has been developed to compute Legendre function values of the first kind. The solution values were computed using a Legendre differential equation, which was transformed into a system of two first order differential equations. The computed values were compared using *Mathcad* and *Derive* software, and it was found that the values matched well with

an error of approximately 10^{-12} . The Joubert-Greeff test for the numerical solutions of ODEs [7] was also employed and it also confirmed that the algorithm developed is good for computing Legendre polynomial values at default machine accuracy.

As an application in physics, the numerical values were applied in the example of sound scattering by a sphere. The quantities that were examined are sound pressure and intensity of the scattered sound wave and it was found that the scattered sound depends on the Legendre polynomials for directivity. The associated Legendre functions are defined in terms of the Legendre functions of the first kind as follows:

$$P_n^m(x) = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} [P_n(x)]. \quad (5.1)$$

Hence, the numerical algorithm developed in this paper could be further extended to compute the associated Legendre function values.

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