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A Shooting Method to Solve Singular Heat Transfer Equation Using Automatic Differentiation

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Abstract: The existence of singularity in the equation need to use specific techniques to solve a solution of the nonlinear two-point boundary value problem that models the steady-state temperature distribution in a cylinder. Taylor series expansion and shooting method have been applied. To obtain the coefficients in the Taylor series expansion, this study uses automatic differentiation the aid of recursive formulas derived from the governing differential equation itself. In addition, this method does not have to carry out lengthy algebraic manipulations for obtaining higher-order derivatives because it is only need to substitute the value in order to find coefficients in the Taylor series expansion. Shooting method is the techniques to solve initial-value problems repeatedly until the boundary conditions is satisfied using MAPLE 18 and are presented in the form of table. The solution of the initial value problem is obtained as a Taylor series expansion of arbitrary order. A solution of the result of Taylor series expansion are depends on heat generation constants (α). The heat generation constants (α) in Taylor series expansion are analyzed and discussed in the form of table and graph. It is found that the difference between α=0.1 until α=0.8 in Taylor series expansion of the equation are too small.

Keywords: Taylor Series Expansion, Shooting Method, Automatic Differentiation

1. Introduction

In science and engineering sector, there have been numerous studies about heat transfer toward steady-state temperature distribution. Based on [1], heat transfer describes the flow of heat (thermal energy) due to temperature differences and the subsequent temperature distribution and changes. Steady-state heat transfer happens when temperature, properties of thermophysical and surface and bulk motion of fluid are constant over time.

Nonlinear two-point boundary value problem that models the steady-state temperature distribution in a cylinder occurs when thermophysical properties are assumed to vary with temperature.

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This problem always happens in real life conditions, however it is more complex to solve. Ha [2] said that the two-point boundary value problems are problems in which, for a set of possibly nonlinear ODE, some boundary conditions are specified at the initial value of independent variable, while the remainder of boundary conditions are specified at the terminal value of the independent variable. If the problem of two-point boundary value problem cannot be solved analytically, then numerical methods can be used to solve the problem. Numerical methods have two types of techniques for solving two-point boundary values problems which are shooting method, (SM) and finite difference method, (FDM). Morrison et al. [3] interpreted that central to a shooting method is the ability to integrate the differential equation as an initial value problem with guesses for the unknown initial values.

Analytical treatment to solve this problem by Kubicek and Hlavacek [4] leading to a closed form solution which means the method used possess no solution. Na and Tang [5] use numerical treatment which is consisted of converting the boundary value problem to a related initial value problem and using runge-kutta method for its solution. This approach requires long computing time and effort. A solution of this problem also often becomes very sensitive to even small change is assumed boundary condition. Recently, this boundary value problem with singularity has been studies by Quartapelle and Rebay [6]. They have been developed a class of multipoint techniques for the solution of this problems that require the formulation of a nonlocal integral condition. These techniques also require a considerable amount of computational effort too.

In order to solve the nonlinear two-point boundary value problem that models the steady-state temperature distribution in a cylinder, SM applied in this study. This method was chosen to solve the boundary value problem in Taylor series expansion. Taylor series expansions is primarily presented in introductory calculus courses but the subject is frequently revisited in numerical methods courses for STEM (Science, Engineering and Mathematics) undergraduates said Pantaleón & Ghosh [7]. Taylor series expansion is used to solve singularity problem in the equation in this study. Taylor series expansion method has been motivated by Stoer and Bulirsch [8]. In order to maintain the simplicity of finding Taylor coefficients, the present study uses Automatic Differentiation, (AD) to find the coefficients in the Taylor series expansion without the requirement to derive the symbolic expressions at any time. AD is a method that will convert the program into a sequence of primitive operations which have specified routines for computing derivatives. In this study, the nonlinear two-point boundary value problem that models the steady-state temperature distribution in a cylinder of unit radius that has singularity problem. In order to establish more efficient approach to this problem, this study is uses Taylor series expansion to obtain the solution. This method has been used by Stoer and Bulirsch [8]. In order to find Taylor coefficients, this study need to drive the symbolic expression at any time which is need to be obtained as part of the solution to solve initial value problem using shooting method. In order to avoid this lengthy symbolic expression, this study uses an automatic AD method to maintain the simplicity of shooting approach and without having to derive the symbolic expression at any time. This study has two objectives which are to find a nonlinear heat transfer equation that has singularity using Taylor series expansion and shooting method and to simplify the method of finding coefficient in Taylor series expansion.

2. Methodology

In this section, the governing equation for nonlinear two-boundary value problem were discussed. Taylor series expansion and shooting method have been applied to describe in more detail. The use of automatic differentiation to find coefficients in Taylor series expansion will also be discussed in further detail.

2.1 Taylor Series Expansion

The equation of steady-state temperature distribution of the two-boundary value problem with the interior cylinder of unit radius is as follows by [9]

$$y'' = -\frac{y'}{x} - f(y), \quad y'(0) = y(1) = 0 \qquad \textit{Eq. 2.1}$$

with $f(y) = \alpha e^{y}$ where $0 < \alpha \le 0.8$

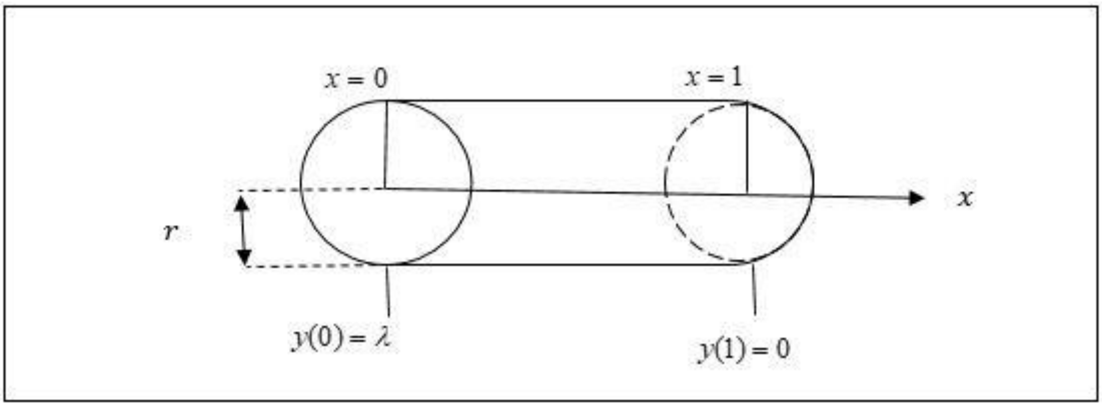

Figure 2.1: Two-boundary value problem for steady-state temperature distribution in the cylinder with unit radius

We write a J th-order of Tayloe series solution for equation (2.1) in the form of

$$y(x) = (y)_0 + \sum_{j=2}^{J} (y)_j x^j \qquad \textit{Eq. 2.2}$$

by using notation of quantity $(y)_j$,

$$(y)_j = \frac{y^j(0)}{j!} \qquad \textit{Eq. 2.3}$$

The $(y)_j$ is the jth Taylor coefficient for $y(x)$ around $x = 0$. The term of $(y)_1 x$ is missing in equation (2.3) because the condition of $y^{'}(0) = 0$ in equation (2.1). Then, this study needs to develop a technique for obtaining $(y)_j$ for $j = 0, 2, 3, .., J$ for an arbitrary J. Differentiate the equation (2.2) yields

$$y^{'}(x) = \sum_{j=2}^{J} j(y)_j x^{j-1} \qquad \textit{Eq. 2.4}$$

Next, divide both side of the equation (2.4) by x yield

$$\frac{y^{'}(x)}{x} = \sum_{j=2}^{J} j(y)_j x^{j-2} \qquad \textit{Eq. 2.5}$$

Substitute $\frac{y^{'}(x)}{x}$ from equation (2.5) into differential equation of (2.1) and rearranging the terms of yields

$$y^{(2)}(x) = -2(y)_2 - \sum_{j=3}^{J} j(y)_j x^{j-2} - f(y(x)) \qquad \textit{Eq. 2.6}$$

Let $x = 0$ and substitute $\frac{y^{(2)}(0)}{2} = (y)_2$ in equation (2.6) and obtain

$$2(y)_2 = -2(y)_2 - f(y(0))$$

After simplification, the equation of $(y)_2$ becomes

$$(y)_2 = -\frac{1}{4} f(y(0)) \qquad \textit{Eq. 2.7}$$

At this point, note that it is convenient to extend the notation of Taylor coefficients for $y(x)$ to $f(y(x))$ as well. So, let

$$(f)_j = \left.\frac{d^j f(y(x))}{dx^j}\right|_{x=0} \qquad \textit{Eq. 2.8}$$

After the notation (2.8), the equation (2.7) can be written as

$$(y)_2 = -\frac{1}{4}(f)_0 \qquad \textit{Eq. 2.9}$$

The jth Taylor coefficients for $y(x)$ around $x = 0$ can be concluded as

$$y^{(m)}(x) = -m(m-2)(m-3)\cdots 2\cdot 1(y)_m - \sum_{j=m+1}^{J} j(j-2)(j-3)\cdots(j-m+1)(y)_j x^{j-m} - \frac{d^{m-2} f(y(x))}{dx^{m-2}} \qquad \textit{Eq. 2.10}$$

m as the order of the yield.

Assume $x = 0$ in the equation (2.10) and substitute $\frac{1}{m!} y^{(m)}(0) = (y)_m$ and $\left.\frac{d^{m-2} f(y(x))}{dx^{m-2}}\right|_{x=0}$ $= (m-2)!(f)_{m-2}$ into equation (2.10)
And becomes

$$[m! + m(m-2)!](y)_m = -(m-2)!(f)_{m-2} \qquad \textit{Eq. 2.11}$$

which yields

$$(y)_m = -\frac{1}{m^2}(f)_{m-2} \qquad \textit{Eq. 2.12}$$

2.2 Automatic Differentiation

An Automatic Differentiation is used to require the following recursive formula for evaluation of successive Taylor coefficients for $f(y) = \alpha e^y$. This rule may be found in Moore [10]. If $u(x)$ is any function of x, then the function get

$$(e^u)_j = \sum_{i=0}^{j-1} (1 - \frac{i}{j})(e^u)_i (u)_{j-i} \qquad \textit{Eq. 2.13}$$

The equation in (2.13) evaluates exact derivatives, it can be obtain using algebraic manipulation of the symbolic expression of the functions. This technique shows how the different Taylor coefficient $(f)_j$ is calculated, so the $(y)_j$ will be determine. This study introduces T as temporary variable and f as the end result of the following sequence of operation. Rewrite the equation $f(y) = \alpha e^y$ as a sequence of calculations that involve arithmetic operation, so the equation in (2.13) for AD can be applied.

$$T = e^y,$$
$$f(y) = \alpha T \qquad \textit{Eq. 2.14}$$

For (2.14) it has $j > 0$

$$(T)_j = \sum_{i=0}^{j-1} (1 - \frac{i}{j})(T)_i (y)_{j-i}$$

$$(f)_j = \alpha (T)_j \qquad \textit{Eq. 2.15}$$

Taylor coefficients in (2.2) are calculated by using

$$(y)_j = \begin{cases} \lambda_0 & \text{for } j = 0 \\ -\frac{1}{j^2}(f)_{j-2} & \text{for} \end{cases} \qquad \textit{Eq. 2.16}$$

2.3 Shooting Method

Shooting Method approach is to determine appreciate set of boundary condition at one end. So, the boundary condition would then be satisfied at the other end. Let $y(0) = \lambda$ as unknown to be determined as part of the solution. If the value of λ determined, the Taylor series expansion for $y(x)$ based on the value of λ. Let $g(\lambda) = y(1;\gamma)$.

For simplicity, assume that this study uses the fourth order Taylor series expansion for $y(x)$ with $y(0) = \lambda$ and obtain

$$y(x;\lambda) = \lambda - \frac{1}{2}\alpha e^{\lambda}\frac{x^2}{2!} + \frac{3}{8}\alpha^2 e^{2\lambda}\frac{x^4}{4!} \qquad \textit{Eq. 2.17}$$

To get the proper value of λ, the nonlinear algebraic equation with $x = 1$ need to solve first

$$y(1) = g(\lambda) = \lambda - \frac{1}{4}\alpha e^{\lambda} + \frac{1}{64}\alpha^2 e^{2\lambda} = 0 \qquad \textit{Eq. 2.18}$$

Let $\gamma = \alpha e^{\lambda}$, equation (2.18) equivalent to

$$\gamma = \alpha e^{-p(\gamma)} \qquad \textit{Eq.2.19}$$

where

$$p(\gamma) = -\frac{1}{4}\gamma + \frac{1}{64}\gamma^2 \qquad \textit{Eq. 2.20}$$

Since γ in equation (2.19) lends itself naturally to fixed-point iteration obtains

$$\gamma_{n+1} = \alpha e^{-p(\gamma_n)}, n = -0,1,2,\ldots, \qquad \textit{Eq. 2.21}$$

Start with the initial guess $\gamma_0 = \alpha e^{\lambda_0}$ and continuing to iterate until $|\gamma_{n+1} - \gamma_n| < \varepsilon$ for some prescribed error tolerance, ε. Once equation (2.19) is solved for the value γ, the proper value of λ can calculated as

$$\lambda = \ln(\frac{\gamma}{\alpha}) \qquad \textit{Eq. 2.22}$$

3. Results and Discussion

In this chapter, the proper value of λ have been determined by applying SM by using the fourth order Taylor series expansion for $y(x)$ in (2.18) generated by using MAPLE 18. The Taylor series expansion for $y(x)$ were successfully generated by using MAPLE 18 based on the value of λ. Then, this study solved the result of $y_J(x;\alpha)$ denote the value of $y(x)$ obtained by using J th-order Taylor series expansion.

3.1 Solving Taylor Coefficients using Automatic Differentiation

The Taylor coefficients, $(f)_j$ on $f(y)=\alpha e^y$ in (2.1) can be recursively computed using (2.16). This study obtained $(y)_5$ until $(y)_{12}$ easily with only substitute the value of j in (2.16) without having derivative symbolic expression. For example, to solve fifth Taylor coefficient for $f(y)$. Firstly, substitute the fifth Taylor coefficient, $(y)_5$ which $j=5$ in (2.16),

$$(y)_5=-\frac{1}{5}(f)_{5-2}$$

After simplification, $(y)_5$ equal to

$$(y)_5=-\frac{f_3}{25} \quad \textit{Eq. 3.1}$$

$$(y)_6=-\frac{f_4}{36} \quad \textit{Eq. 3.2}$$

$$(y)_7=-\frac{f_5}{49} \quad \textit{Eq. 3.3}$$

$$(y)_8=-\frac{f_6}{64} \quad \textit{Eq. 3.4}$$

$$(y)_9=-\frac{f_7}{81} \quad \textit{Eq. 3.5}$$

$$(y)_{10}=-\frac{f_8}{100} \quad \textit{Eq. 3.6}$$

$$(y)_{11}=-\frac{f_9}{121} \quad \textit{Eq. 3.7}$$

$$(y)_{12}=-\frac{f_{10}}{144} \quad \textit{Eq. 3.8}$$

3.2 Finding λ as Unknown for Obtain the Taylor Series Expansion for $y(x)$ using Shooting Method

In order to solve this, this study started with the initial guess $\gamma_0=\alpha e^{\lambda_0}$ with $\lambda_0=0.2$ and $\alpha=0.8$. After γ_0 obtain, substitute the value of γ_0 in equation (2.20) and continuing to iterate until $|\gamma_{n+1}-\gamma_n|<\varepsilon$ for some prescribed error tolerance, $\varepsilon=10^{-8}$.

Table 3.1: Shooting method iteration until $|\gamma_{n+1}-\gamma_n|<\varepsilon$

n	γ_n	$p(\gamma)$	$\lvert\gamma_{n+1}-\gamma_n\rvert<\varepsilon$
0	0.9771222064	-0.2293623046	
1	1.006238130	-0.2357389829	0.3702057824
2	1.012675088	-0.2371451652	0.006436958
3	1.014100095	-0.2374562894	0.001425007

4	1.014415656	-0.2375251777	0.000315561
5	1.014485539	-0.2375404331	0.000069883
6	1.014501016	-0.2375438116	0.000015477
7	1.014504443	-0.2375445598	0.000003427
8	1.014505202	-0.2375447254	0.000000759
9	1.014505370	-0.2375447621	0.000000168
10	1.014505408	-0.2375447704	0.000000038

The iteration stops at $|\gamma_{10}-\gamma_9|<\varepsilon$ which is $p(\gamma)=-0.2375447621$ and then substitute the value of $p(\gamma)$ into (2.19),

$$\gamma=(0.8)e^{-(-0.2375447621)}$$

And obtained $\gamma=1.014505408$.
Continue to the next step that need to substitute the value of γ into (2.22),

$$\lambda=\ln\left(\frac{1.014505408}{0.8}\right)$$

And obtained $\lambda=0.2375447623$. In order to obtain the value of $p(\gamma)$, MAPLE 18 is used for the iteration in Table 3.1.

3.3 The Result $y_J(x;\alpha)$ Denote the Values of $y(x)$ Obtain by Using the J th-order Taylor Series Expansion

Let $y_J(x;\alpha)$ the value for $y(x)$ obtained using the J th-order Taylor series expansion based on the value of λ, when $0<\alpha\le 0.8$ and $x=0$ to $x=1$ in steps of 0.1. $y_{12}(x;\alpha)$ obtained.

$$\begin{aligned} y_{12}(x;0.4) &= 0.2375448-0.1268132x^2-0.0220225x^4-0.0108691x^6 \\ &\quad -0.0061824x^8-0.0039753x^{10}-0.0027668x^{12} \end{aligned} \qquad \textit{Eq. 3.9}$$

Table 3.2: The solution of $y_{12}(x)$ for $0 < \alpha \le 0.8$

x	$y_{12}(x;0.1)$	$y_{12}(x;0.2)$	$y_{12}(x;0.3)$	$y_{12}(x;0.4)$	$y_{12}(x;0.5)$	$y_{12}(x;0.6)$	$y_{12}(x;0.7)$	$y_{12}(x;0.8)$
0.0	0	0	0	0	0	0	0	0
0.1	0.009999392	0.009998821	0.009998287	0.009996108	0.0099961	0.009996108	0.009996108	0.009996108
0.2	0.039990131	0.039980869	0.039972185	0.039937106	0.0399371	0.039937106	0.039937106	0.039937106
0.3	0.089948834	0.089900751	0.089855608	0.089675955	0.0896760	0.089675955	0.089675955	0.089675955
0.4	0.159832546	0.159674901	0.159526598	0.158947686	0.1589477	0.158947686	0.158947686	0.158947686
0.5	0.249571193	0.249166530	0.247327017	0.247327017	0.2473270	0.247327017	0.247327017	0.247327017
0.6	0.359052740	0.358156080	0.354135479	0.354135479	0.3541355	0.354135479	0.354135479	0.354135479
0.7	0.488093741	0.486282490	0.478239948	0.478239948	0.4782399	0.478239948	0.478239948	0.478239948
0.8	0.636379803	0.632924442	0.617620284	0.617620284	0.6176203	0.617620284	0.617620284	0.617620284
0.9	0.803345204	0.796960087	0.768462162	0.768462162	0.7684622	0.768462162	0.768462162	0.768462162
1.0	0.987933642	0.976289414	0.923315122	0.923315122	0.9233151	0.923315122	0.923315122	0.923315122

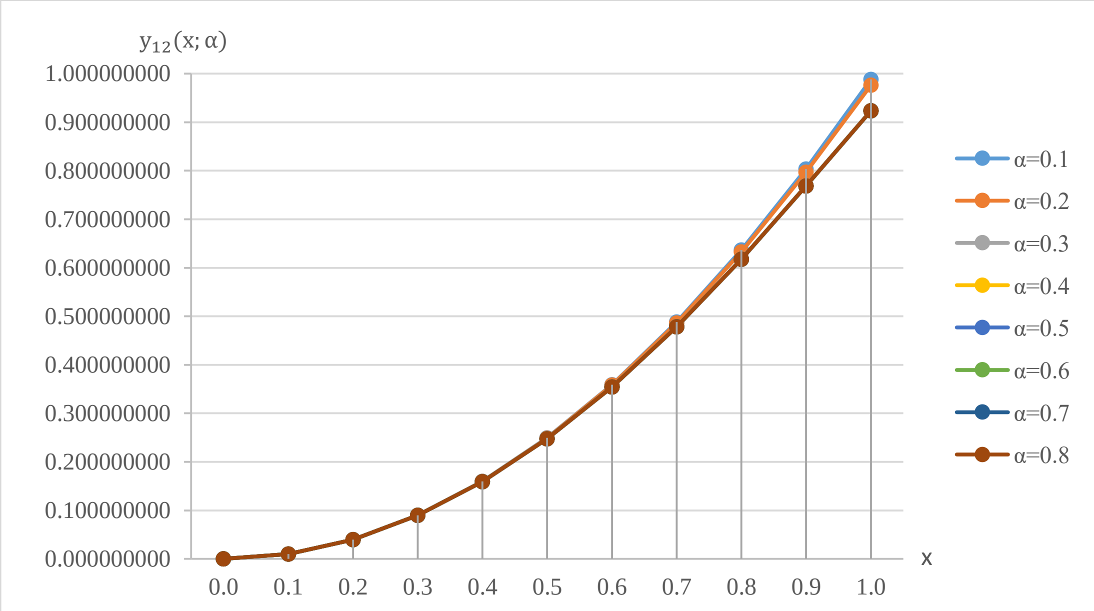

Figure 3.1: Graph of the solution of $y_{12}(x)$ for $0 < \alpha \leq 0.8$

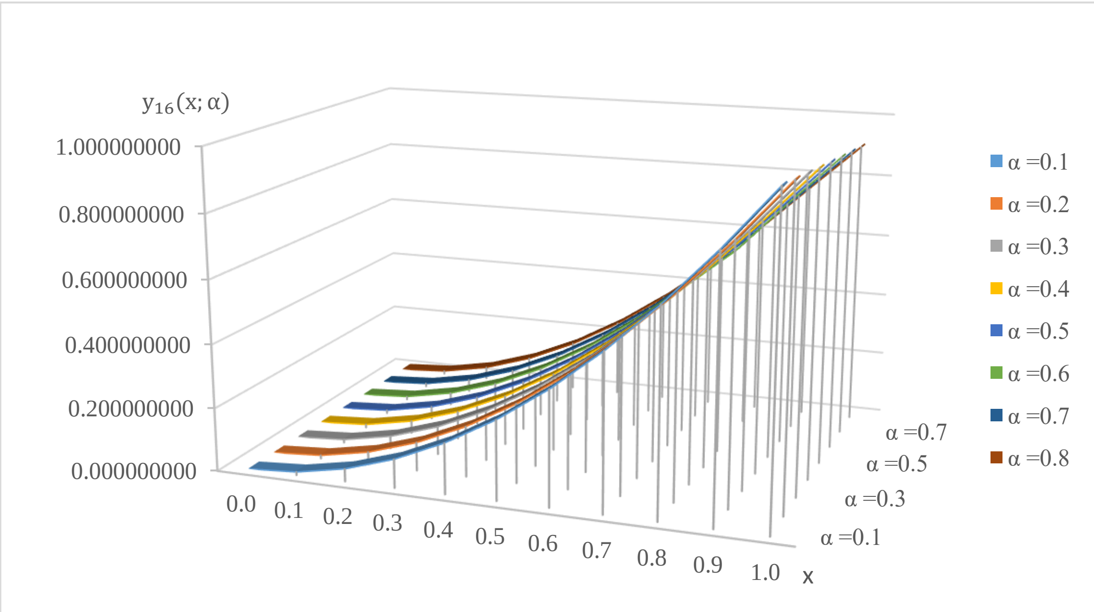

Figure 3.2: 3D-graph of the solution of $y_{12}(x)$ for $0 < \alpha \leq 0.8$

From the Table 3.2, shows the solution of $y_{12}(x)$ for the parameter $x = 0$ to $x = 1$ in steps of 0.1 obtained by J th-order Taylor series expansion. For, Figure 3.1 this study used the line graph to show the solution obtained by the solution of $y_{12}(x)$ for $0 < \alpha \leq 0.8$ using Microsoft Excel. Thus, the difference between $y_{12}(x;0.1)$ and $y_{12}(x;0.8)$ are too small based on the graph in Figure 3.1. The difference between $y_{12}(x;0.1)$ and $y_{12}(x;0.8)$ can be seen more clearly based on Figure 3.2.

This study has successfully applied the present method of Stoer and Burlisch [8]. This study has applied a SM to obtain the Taylor series expansion for the solution that have singularity, nonlinear equation two-boundary value problem of steady-state temperature distribution in the interior cylinder with unit radius. After this study solved the initial value problem just once, the unknown boundary condition at one end can be obtained. The coefficients of Taylor series expansion needed to describe the nonlinear algebraic equation to find the proper initial condition is also derived. Fixed-point iteration is used to solve this nonlinear equation.

4. Conclusion

As a conclusion, the objectives of this research have been achieved. This study obtains the value for $y(x)$ of nonlinear heat transfer that has singularity by using Taylor series expansion in (3.9) based on the result in Table 3.2. The result in Table 3.2 is represents the value of λ that have been obtained by using SM. For the second objective, this study has obtained Taylor coefficients for the function $f(y)$ using AD method without driving symbolic expression for the derivatives and the solution shown in (3.1) until (3.8). In the future, some recommendations for the next researcher are to choose a smaller step size of $0 \le x \le 1$ for solve $y_{12}(x)$ to obtain more accurate solution and choose higher J th-order Taylor series expansion for $y_J(x;\alpha)$ to obtain $y(x)$. The higher value J th-order Taylor series expansion, the higher the difference can be seen between $y_J(x;0.1)$ and $y_J(x;0.8)$.

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