# Shooting methods for solving eigenvalue problem

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## 1 Two-points boundary problem

This note is based on Ref. [1], where the authors describe what is two-points boundary problem and how to attack it numerically. The two-points boundary problem is usually written in the following standard form:

$$\frac{dy_i}{dx} = g_i(x, y_1, y_2, \ldots, y_N), \quad i = 1, 2, \ldots, N \tag{1}$$

$$B_{ja}(x_a, y_1(x_a), y_2(x_a), \ldots, y_N(x_a)) = 0, \; j = 1, 2, \ldots, n_1 \tag{2}$$

$$B_{kb}(x_b, y_1(x_b), y_2(x_b), \ldots, y_N(x_b)) = 0, \; k = 1, 2, \ldots, n_2 \tag{3}$$

where $n_1 + n_2 = N$, $x_a$ and $x_b$ are two boundary points which are not equal to each other.

### 1.1 Problem that can be reduced to the standard form

As is known to us, any second-order differential equation can be rewritten as two first-order differential equations by introducing the derivative of the unknown function as a new unknown function. Next, consider whether eigenvalue problems of second-order differential equation can be rewritten in the standard form of two-points boundary problem. As an example, consider the following eigenvalue problems:

$$\frac{d}{dx}\left(x^3 \frac{du}{dx}\right) + \lambda x u = 0, \tag{4}$$

with the boundary conditions

$$u(1) = 0, \tag{5}$$
$$u(2) = 0. \tag{6}$$

Define the eigenvalue $\lambda$ as a new function $y_3 = \lambda$, then $y_3$ satisfies the following equation

$$\frac{dy_3}{dx} = 0. \tag{7}$$

As usual, define two functions $y_1 \equiv u$, $y_2 \equiv du/dx$, then Eq. (4) is written as

$$\frac{dy_1}{dx} = y_2, \tag{8}$$

$$\frac{dy_2}{dx} = -\frac{y_3}{x^2} y_1 - \frac{3}{x} y_2, \tag{9}$$

The boundary condition now is written as $y_1(x=1) = 0$, $y_1(x=2) = 0$. However, in this case, we have three unknown functions but only two boundary conditions. It is obvious that we need to specify a third boundary condition to make this problem take the standard form given by Eqs. (1)-(3). Note that Eq. (4) is linear and homogeneous. Further note that the value of $u$ at the two boundary points are all zero. It follows that any solution to Eq. (4) multiplied by a constant factor satisfies both Eq. (4) and the boundary conditions. This means the derivative of $u$ (i.e., $y_2$) at the boundary points can take any nonzero values (since the derivative of $cu$ is equal to $c du/dx$, and the constant $c$ can be chosen to adjust the value of the derivative). Therefore, the boundary condition of $y_2$ at $x = 1$ can be chosen to be an arbitrary nonzero value. Thus, the desired third boundary condition is obtained and the eigenvalue problem is written in the standard form of the two-points boundary problem.

## 1.2 Numerical methods

One obvious numerical method to solve the two-points boundary problem is the shooting method. The code implementing this method involves an ordinary differential equation integrator and a root finder for nonlinear algebra equations. Refer to Ref. [1] for the details of the shooting method.

## 1.3 Numerical results

Next, I give the numerical results of Eqs. (4)-(6) obtained by using the shooting method. In fact, the eigenvalues and eigenfunctions for Eqs. (4)-(6) can be obtained analytically, which is given respectively by

$$\lambda_n = 1 + \left(\frac{n\pi}{\ln 2}\right)^2, n = 1, 2, 3..., \tag{10}$$

and

$$y_n(x) = \frac{1}{x}\sin\left(\frac{n\pi}{\ln 2}\ln(x)\right). \tag{11}$$

The numerical results obtained by using the shooting method is plotted in Fig. 1. Also plotted in the figure is the analytical eigenfunction given by Eq. (11) with $n = 2$. The results indicate that the numerical solution agree well with the analytical results. (Numerical codes are located in /home/yj/project/shooting_method/.)

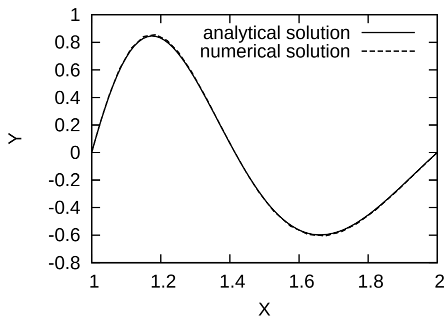


**Figure 1.** Numerical eigenfunction obtained by the shooting method. The eigenvalue obtained is $\lambda = 83.168732$, which corresponds to $n = 1.999995$ in Eq. (10). Also plotted in the figure is the analytical eigenfunction given by Eq. (11) with $n = 2$. Note that the numerical solution and the analytical one agree with each other so well that they are indistinguishable at this scale. We have scaled the numerical results by a constant factor to make it match the analytical solution (this is justified since an eigenfunction multiplied by any constant is still an eigenfunction).

Next, consider the Hermite differential equation

$$u_{xx} + (\lambda - x^2)u = 0 \tag{12}$$

with the boundary conditions

$$u(+\infty) = 0, u(-\infty) = 0. \tag{13}$$

Define $y_1 = u$, $y_2 = du/dx$, $y_3 = \lambda$, then Eq. (12) can be put in the following standard two-points boundary problem

$$\frac{dy_1}{dx} = y_2$$

$$\frac{dy_2}{dx} = -(y_3 - x^2)y_1$$

$$\frac{dy_3}{dx} = 0.$$

In numerical treatment, the infinite boundaries must be truncated to form a finite interval. In practice, approximate boundary points $x_a = -5$ and $x_b = 5$ can be good for the Hermite differential equation. Then the boundary conditions become $y_1(-5) = 0$, $y_1(5) = 0$, and $y_2(-5)$ can be chosen to be an arbitrary nonzero value.

Next, I will give the numerical solution of Eq. (12)-(13). In fact the eigenvalues and eigenfunctions for Eq. (12)-(13) can be obtained numerically, which is given respectively by

$$\lambda = 2n + 1, n = 0, 1, 2, ... \tag{14}$$

$$h_n(x) \equiv \frac{1}{\pi^{1/4}\sqrt{2^n n!}} \exp\left(-\frac{x^2}{2}\right) H_n(x), \tag{15}$$

where

$$H_n(x) = (-1)^n \exp(x^2) \left(\frac{d}{dx}\right)^n \exp(-x^2). \tag{16}$$

Figure 2 plots the numerical result obtained by using the shooting method.

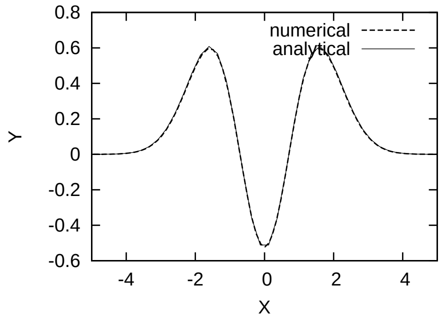


**Figure 2.** Numerical eigenfunction obtained by the shooting method for Eq. (12) with the boundary condition $y(-5) = 0$ and $y(5) = 0$. The eigenvalue obtained is $\lambda = 5.00000$. Also plotted in the figure is the analytical eigenfunction given by Eq. (15) with $n = 2$. Note that the curves of the numerical solution and the analytical one agree with each other so well that they are almost indistinguishable at this scale. The numerical results have been scaled by a constant factor to make it match the analytical solution (this is justified since an eigenfunction multiplied by any constant is still an eigenfunction)

Next, consider a singular Sturm-Liouville eigenvalue equation:

$$\frac{d}{dx}\left[(\omega - x)\frac{dy}{dx}\right] + (\omega - x)\, y = 0, \tag{17}$$

with the boundary condition

$$y(0) = 0, y(1) = 0. \tag{18}$$

An Sturm-Liouville equation is said to be "singular" if the coefficients have singularities. In the present case, the singularity refers to that the coefficients before the highest order derivative is zero at the location $x = \omega$. This singularity can be more obvious if we write Eq. (17) in the standard form of the two-points boundary problem, which is given by

$$\frac{dy_1}{dx} = y_2 \tag{19}$$

$$\frac{dy_2}{dx} = -y_1 + \frac{y_2}{y_3 - x} \tag{20}$$

$$\frac{dy_3}{dx} = 0. \tag{21}$$

where, as usual, $y_1$, $y_2$, and $y_3$ are defined respectively by $y_1 = y$, $y_2 = dy/dx$, and $y_3 = \omega$. Note that the range of $x$ is $[0, 1]$. If $y_3$ happens to be also in this range, the last term in Eq. (20) will become infinite. It can be proved analytically that every value in the range [0, 1] will be an eigenvalue of Eqs. (17)-(18) and the corresponding eigenfunction will have singularity in the location where $\omega - x = 0$ (I do not prove this analytically). This means the range [0, 1] is the continuous spectrum of this eigenvalue problem. Now comes the question: how to obtain numerically the eigenvalues in the range of the continuous spectrum and the corresponding eigenfunctions by using the shooting method? The difficulty arises from the last term in Eq. (20), which will become infinite at one location within the integration path when Eq. (20) in integrated from $x_a = 0$ to $x_b = 1$. A rough method to avoid this difficulty is to use a fixed step size ODE integrator and coarse grids that no grid point happens to exactly locate at the point where $\omega - x = 0$. The essence of this method is to use numerical discrete to eliminate the singularity of the equation. The Numerical results for eigenvalue problem in Eqs. (19)-(21) obtained by this method is plotted in Fig. 3.

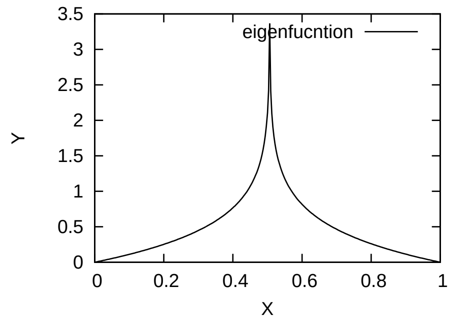


**Figure 3.** The eigenfunction corresponding to the eigenvalue $\omega = 0.50157022$ obtained by using the shooting method. The singularity about at $x = 0.5$ is obvious. Also note that the singularity is of the $\ln|x - x_0|$ type. A simple Euler integrator with step size 1./320 is used to integrate Eqs. (19)-(21) from $x_a = 0$ to $x_b = 1$.

# Bibliography

**[1]** W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. *Numerical Recipes in Fortran 77*. Cambridge University Press, Cambridge, UK, 1992.