Shooting method for solving boundary value problems

Shubham Raghuvanshi
Harish Chandra Research Institute

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Solution of initial value problems

- An m'th order ordinary differential equation of the form

$$\frac{d^m y(t)}{dt^m} = f\left(t, y(t), \frac{dy(t)}{dt}, \frac{d^2 y(t)}{dt^2}, ..., \frac{d^{m-1} y(t)}{dt^{m-1}}\right) \tag{1}$$

can be converted to a system of 'm' coupled first order differential equations

$$\frac{dy^{(n-1)}(t)}{dt} = y^{(n)}(t) \ , \ m \geq n \geq 1 \tag{2}$$

by defining 'm+1' new variables $y^{(n)}(t)$, $0 \leq n \leq m$ such that

$$y^{(0)}(t) = y(t) \tag{3}$$

$$y^{(m)}(t) = f(t, y^{(0)}, y^{(1)}, y^{(2)}, ..., y^{(m-1)}) \tag{4}$$

Which can be uniquely solved given 'm' initial conditions of the form

$$y^{(n)}(t_0) = a_n \ , \ 0 \leq n \leq m-1 \tag{5}$$

Methods of numerically solving IVP

Following are some of the well known methods for numerically solving IVP of the form

$$\frac{dy}{dx} = f(x, y) \tag{6}$$

- Euler's explicit and implicit method (Taylor series method of order 1)

$$y_{n+1} = y_n + \Delta x f(x_n, y_n) + O(\Delta x^2) \tag{7}$$

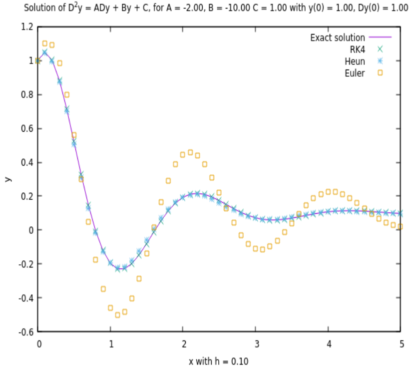
$$y_{n+1} = y_n + \Delta x f(x_{n+1}, y_{n+1}) + O(\Delta x^2) \tag{8}$$

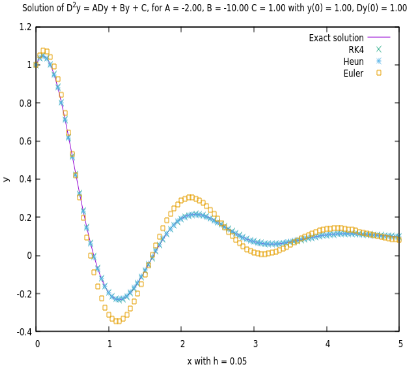
$$y_{n+1} = y_n + \frac{\Delta x}{2}\left(f(x_{n+1}, y_{n+1}) + f(x_n, y_n)\right) + O(\Delta x^3) \tag{9}$$

- Higher-order Taylor series methods
- N^{th} order Runge-Kutta (RKN) methods.

$$y_{n+1} = y_n + \sum_{i=1}^{N} w_i k_i,\ k_i = h_n f\left(x_n + \alpha_i h_n, y_n + \sum_{j=1}^{i-1} \beta_{ij} k_j\right) \tag{10}$$

- Predictor corrector methods


Solution of D^2y = ADy + By + C, for A = -2.00, B = -10.00 C = 1.00 with y(0) = 1.00, Dy(0) = 1.00
Exact solution
RK4
Heun
Euler
y
x with h = 0.10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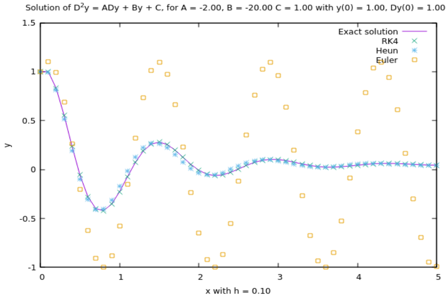
Exact solution
RK4
Heun
Euler
y
x with h = 0.05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Exact solution
RK4
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y
x with h = 0.10

Shooting method for solving second order BVP

Consider a second order BVP

$$y''(x) = f(x, y(x), y'(x)) \ , \ y(x_0) = y_0, y(x_1) = y_1 \tag{11}$$

Let $y(x; a)$ be the solution of the IVP

$$y''(x) = f(x, y(x), y'(x)) \ , \ y(x_0) = y_0, y'(x_0) = a \tag{12}$$

Shooting method solves the BVP by finding the roots of the function

$$F(a) = y(x_1, a) - y_1 \tag{13}$$

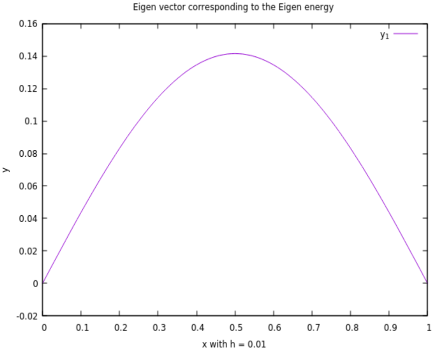
The equation above can be solved numerically using any of numerical techniques such as Mid point method, Secant method etc. The shooting variable here is $y'(0)$, however it can be some other parameter as well e.g. $y(0)$ or Eigen values of TISE,

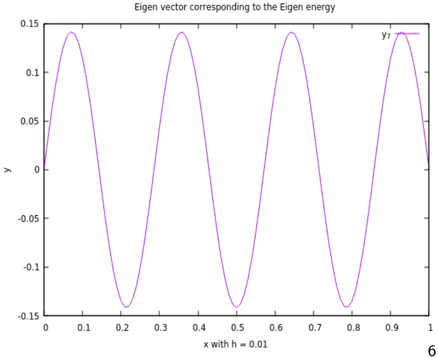
Application: Particle in a box

The TISE for particle in a 1D infinite potential well can be written as a BVP

$$\frac{d^2\psi(x)}{dx^2} = -E\psi(x)\ ,\ \psi(0) = \psi(L) = 0 \tag{14}$$

$E_n = n^2\pi^2$ are the eigenvalues. In order to solve for eigenfunctions one can fix $\psi(0), \psi'(0)$ and treat E as the shooting parameter.





Application: Quantum Harmonic Oscillator

The TISE can be written as a BVP

$$\frac{d^2\psi(x)}{dx^2} = (x^2 - E)\psi(x) \ , \tag{15}$$

Where the boundary conditions for odd and even solutions are $\psi_{odd}(0) = 0, \psi_{odd}(\infty) = 0$ and $\psi'_{even}(0) = 0, \psi_{even}(\infty) = 0$.The eigenvalues are $E_n = 2n + 1$.