
Ch. 08
Ordinary Differential Equations (ODE)
[Boundary Value Problems]

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Two-Point Boundary Value Problems (BVP)

- When ODE are required to satisfy boundary conditions at more than one value of the independent variable, the resulting problem is called a *two point boundary value problem*.
- The most common case is when boundary conditions are supposed to be satisfied at two points — usually the starting and ending values of the integration.
- Unlike IVP, in BVP the boundary conditions at the starting point do not determine a unique solution to start with, and only certain (unknown) values will satisfy the boundary conditions at the other specified point.
- An iterative procedure is required and, for this reason, two point BVP require considerably more effort to solve than do IVP.
- You have to integrate your differential equations over the interval of interest, or perform an analogous “relaxation” procedure, at least several, and sometimes very many, times.
- Only in the special case of linear differential equations you can say in advance just how many such iterations will be required.

Boundary Value Problems: Definition

- The standard two point BVP has the following form: **we seek for the solution to a set of N coupled first-order ODE, satisfying n_1 boundary conditions at the starting point a , and a remaining set of $n_2 = N - n_1$ boundary conditions at the final point b .** (Recall that all differential equations of order higher than first can be written as coupled sets of first-order equations).

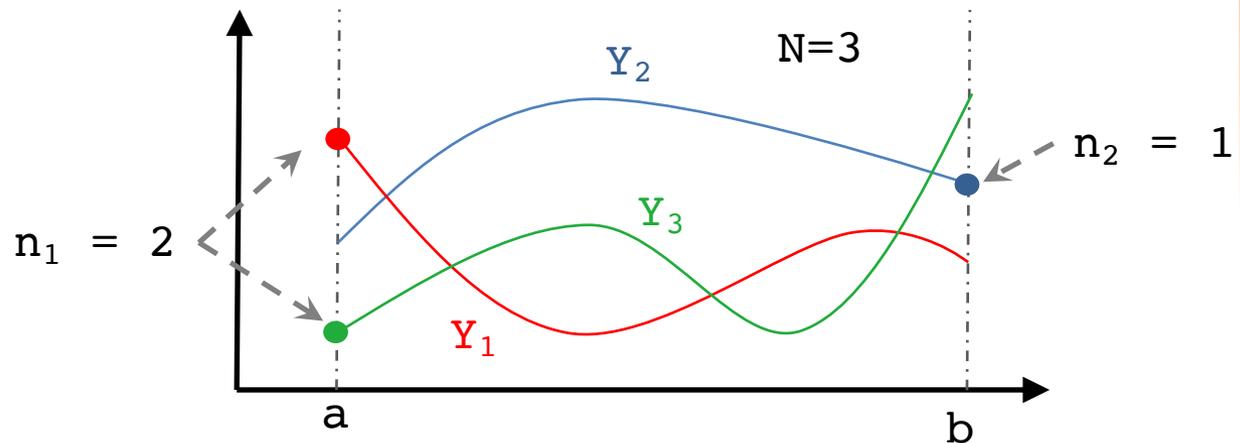
- The ODE are
$$\frac{dY_i}{dx} = R_i(x, \vec{Y}), \quad i = 1, \dots, N$$

which are required to satisfy

$$Y_j = Y_j(a) = \alpha_j, \quad j = 1 \dots n_1$$

$$Y_k = Y_k(b) = \beta_k, \quad k = n_1 + 1 \dots N$$

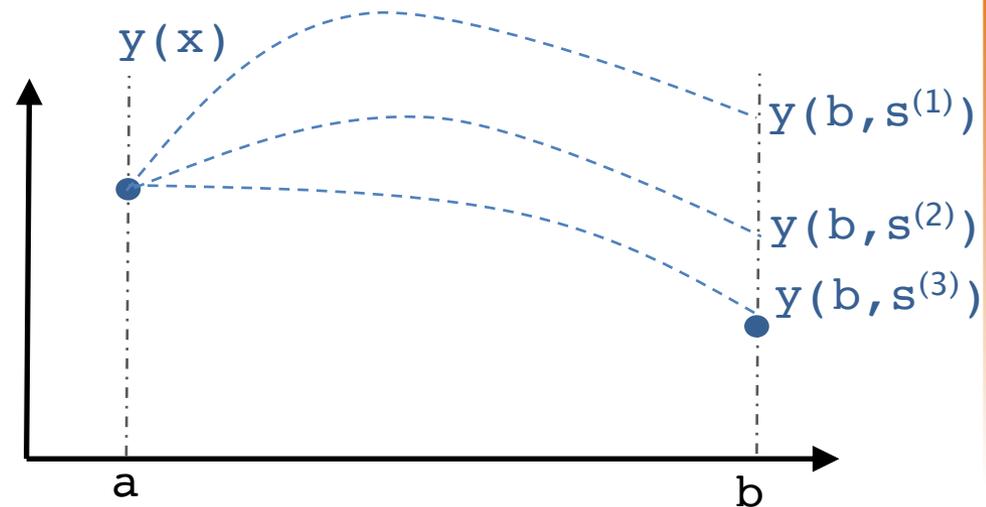
- Here's an example with $N=3$:



Single Shooting Method for BVP

- Consider the simple BVP $\frac{d^2y}{dx^2} = f(x, y, y')$, with $y(a) = \alpha, y(b) = \beta$
- A general strategy for solving a BVP is an iterative one: we guess a trial value for the derivative $s = dy/dx$ at the starting point a and generate a solution by integrating the ODE as an IVP.

- If the resulting solution does not satisfy the b.c., we change the trial value s and iterate again, repeating the process until the b.c. are satisfied within a given tolerance.



- This is the shooting method.

Single Shooting Method for BVP

- Since for each trial value s of the derivative we generate, at the end of integration, a different function $y(b, s)$.
- Requiring that $y(b, s) = \beta$ turns the BVP into a root-finder problem:

$$F(s) = y(b, s) - \beta$$

- If the BVP has a solution, then $F(s)$ has a root.
- Note that Newton-Raphson is inappropriate since we cannot differentiate explicitly the resulting function with respect to k .
- Bisection, False Position or secant may be more appropriate.

BVP: Eigenvalue Problem

- A different variant of the BVP is given by an equation linear equation of the form

$$\frac{d^2y}{dx^2} = f(y, \lambda), \quad \text{with } y(a) = \alpha, y(b) = \beta$$

where λ is a free (unknown) parameter. The problem is overdetermined and there is no general solution for arbitrary values of λ .

- However, for certain special values of λ , the ODE does have a solution: this is the eigenvalue problem for differential equation.

- A typical example is that of a standing wave (a whirling string or rope) fixed at both ends.

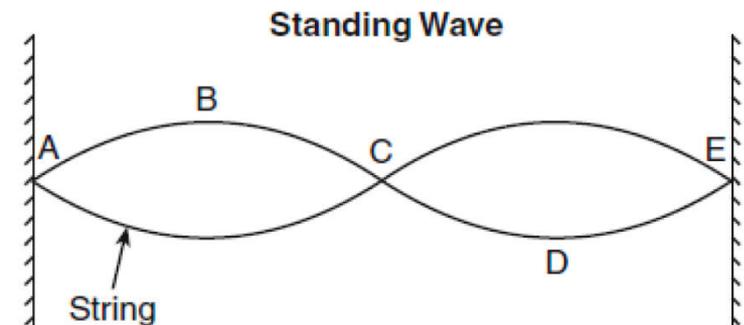
Here the the function is governed by the BVP

$$\frac{d^2\varphi}{dx^2} = -k^2\varphi \quad \text{with } \varphi(0) = 0, \varphi(1) = 0$$

where φ has conditions specified at the boundaries of the independent variable.

- Solutions are possible only for discrete values of k (the eigenvalue):

$$y(x) = \sin(kx), \quad k = n\pi$$



BVP: Eigenvalue Problem

- Eigenvalue problems can also be solved by means of the shooting method.
- Many physical problems can cast as linear homogenous second-order ODE depending on an unknown parameter.
- The stationary Schrodinger equation is an example:

$$\frac{d^2\psi}{dx^2} + k^2(x)\psi = 0 \quad \text{where} \quad \begin{cases} k^2(x) = \frac{2m}{\hbar^2} [E - V(x)] \\ \psi(a) = 0, \psi(b) = 0 \end{cases}$$

Solutions are possible only for certain value of E (the eigenvalue): the eigenfunction (ψ) will oscillate in the classically allowed region where $E > V(x)$ and behave exponentially in the classical forbidden region ($E < V(x)$).

- Other well-known eigenvalue problems are the stationary vibration of a circular membrane, dispersion relations in fluid dynamics, wave propagation, etc...

BVP: Eigenvalue Problem

- Note that for linear homogenous equations (as it is the case for several problems)

$$\frac{d^2y}{dx^2} + k^2(x)y = 0 \quad \text{with} \quad y(a) = \alpha, y(b) = \beta$$

the solution can always be rescaled by an arbitrary multiplicative constant and the normalization of the solution is not specified.

- In these cases, the value of the derivative ($s=dy/dx|_a$) is arbitrary and cannot be used to generate different solutions.
- Instead, we take the eigenvalue k as our free parameter and obtain trial solutions for different values of k until the b.c. are satisfied.

$$F(k) = y(b, k) - \beta$$

- Where $y(b, k)$ means “the solution generate by integrating the ODE from a to b using a trial value k ”

Practice Session #1

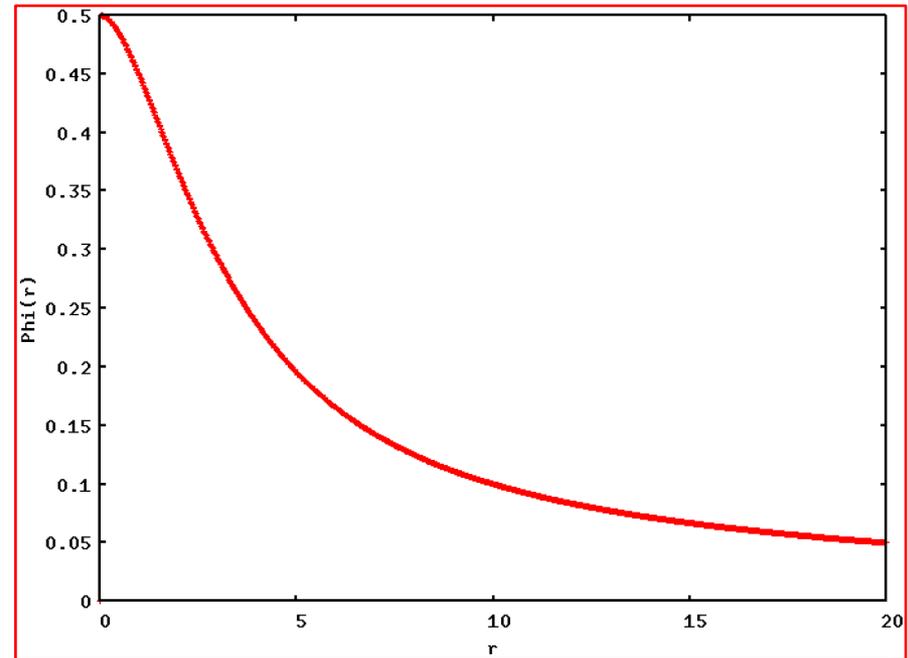
- **poisson.cpp**: we first consider a simple BVP problem given by the 1D spherically symmetric Poisson equation: we wish to find the electrostatic potential Φ generated by a localized charge distribution $\rho(r)$:

$$\nabla^2 \Phi = -4\pi\rho \quad \rightarrow \quad \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\Phi}{dr} \right) = -4\pi\rho \quad (\text{with } \rho(r) = \frac{1}{8\pi} e^{-r})$$

- In order to avoid dealing with the singularity at the origin we use the standard substitution

$$\Phi = \frac{\varphi}{r} \quad \rightarrow \quad \frac{d^2 \varphi}{dr^2} = -4\pi r \rho$$

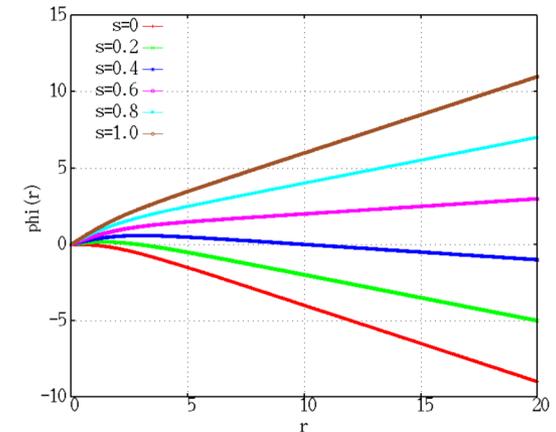
- Boundary conditions are imposed by requiring regularity of the solution:
 - At small r , the potential should vanish
 $\rightarrow \varphi = 0$ at $r=0$
 - At large r , the potential should behave as $1/r \rightarrow \varphi = 1$ at $r=b$
(use $b = 20$ or more)
- The value of the derivative $s = d\varphi/dr$ at $r = 0$ should be used as our free parameter.



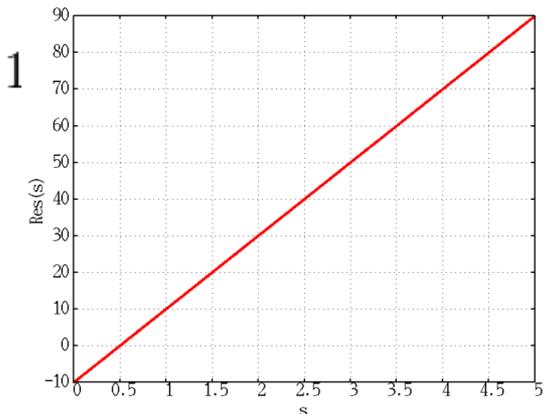
Practice Session #1 (cont)

We proceed step by step:

1. Generate solutions for different values of $s = 0, 0.2, 0.4, 0.6, 0.8, 1.0$ (the first derivative) by integrating the regularized ODE from $r = 0$ to $r = b = 20$ using RK4 (or similar) using 1000 points. Plot the solutions $\varphi(r, s)$ that you have obtained.



2. Implement the residual function, $\text{Residual}(s) = \varphi(b, s) - 1$ [suggested prototype: `double Residual (double)`] and produce a plot of the residual as a function of s in $[0, 5]$. Can you approximately identify the root?



3. Now use bisection or false position to refine the root s for which the residual vanishes. Make sure to supply a range in which the residual changes sign.

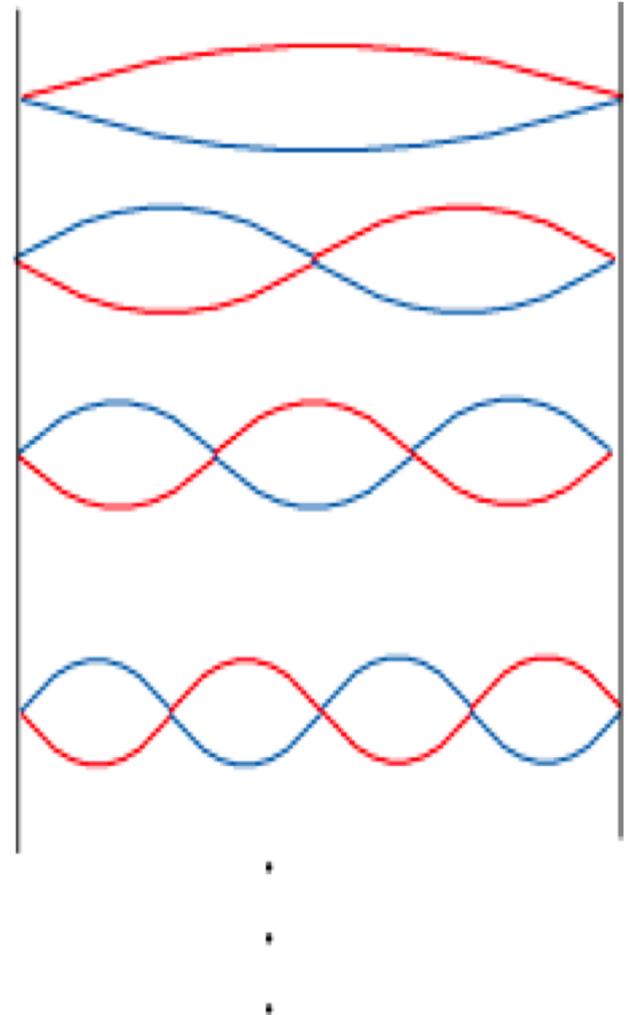
4. Compare your results against the analytical solution:
$$\varphi(r) = 1 - \frac{1}{2}(r + 2)e^{-r}$$

Practice Session #2

- **wave.cpp**: solve the eigenvalue problem

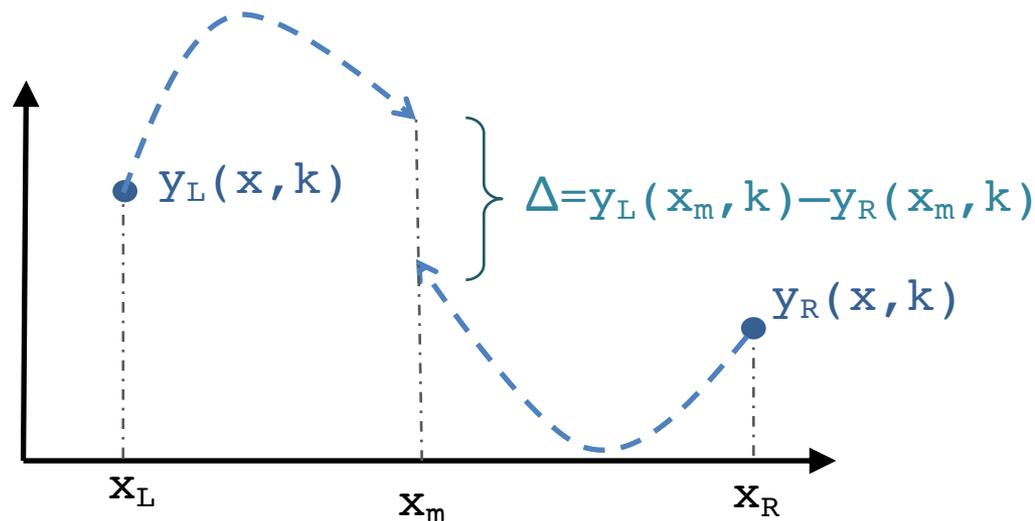
$$\frac{d^2\varphi}{dx^2} = -k^2\varphi \quad \text{with} \quad \varphi(0) = 0, \varphi(1) = 0$$

1. start with a single forward integration from $x=0$ to $x=1$ using 100 points, $k=1$ and $s = dy/dx|_0=1$ (this is completely arbitrary). The code should contain, at this stage, only one single loop. The solution will largely overshoot the final value.
2. modify the code to loop over $k=1,2,3,4,5$ and generate 5 corresponding blocks to be plotted. Use gnuplot to verify that the actual solution lies between $k = 3$ and $k = 4$
3. Move the integration to a function of the type `double Residual(double)` that we will later use for Bisection. Now use Bisection to find the first zero (π).
4. Add a preliminary search using `Bracket()` and then find all of the zeros between 1 and 20.



Integrating to a Matching Point

- In some cases, the two solutions of the 2nd order ODE may be very different. A typical circumstance occurs when the solution, owing to inevitable numerical approximations, contain small admixtures of exponential growing and decaying functions.
- In such cases, it is more convenient to integrate from both ends up to a common point. Two numerical solutions must be generated: a forward integration starting at x_L and a backward integration starting x_R . Both integration stops at the “matching point” x_m which is conveniently chosen by the user.



- At the matching point, we could compute the residual function as the difference between these two solutions: $\Delta = y_L(x_m, k) - y_R(x_m, k)$

Integrating to a Matching Point

- For linear problems, however, the two functions y_L and y_R may differ up to a multiplicative constant, so the residual is better constructed by matching the logarithmic derivative:

$$\left. \frac{y'_L}{y_L} \right|_{x_m} = \left. \frac{y'_R}{y_R} \right|_{x_m} \quad \rightarrow \quad \text{Res}(k) = \frac{y'_L(x_m, k) y_R(x_m, k) - y'_R(x_m, k) y_L(x_m, k)}{D}$$

where D is a normalization factor (if you have no clue, use $D = 1$).

- Thus we have again root-finding problem in the residual.
- Note that results must be independent on the choice of the matching point x_m .

Example: Quantum Eigenvalue Problem

- If a particle of energy E moving in one dimension experiences a potential $V(x)$, its wave function is determined by an ODE (a PDE if greater than 1-D) known as the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).$$

- Setting $\kappa^2 = -\frac{2m}{\hbar^2}E = \frac{2m}{\hbar^2}|E|$, we obtain $\frac{d^2\psi(x)}{dx^2} - \frac{2m}{\hbar^2}V(x)\psi(x) = \kappa^2\psi(x)$.
- For a bounded particles, the wave function must decay exponentially as $|x| \rightarrow \infty$.
- Although it is straightforward to solve the previous ODE with the techniques we have learned so far, we must also require that the solution $\psi(x)$ simultaneously satisfies the boundary conditions at infinity.
- This extra condition turns the ODE problem into an *eigenvalue problem* that has solutions (*eigenvalues*) for only certain values of the energy E .
- The ground-state energy corresponds to the most negative eigenvalue. The corresponding $\psi(x)$ is our eigenfunction.

Practice Session #3

- **qho.cpp**: find the eigenvalues of the quantum harmonic oscillator,

$$-\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi, \quad \text{with} \quad V(x) = \frac{1}{2}kx^2$$

- Rewrite the equation in a more suitable dimensionless form:

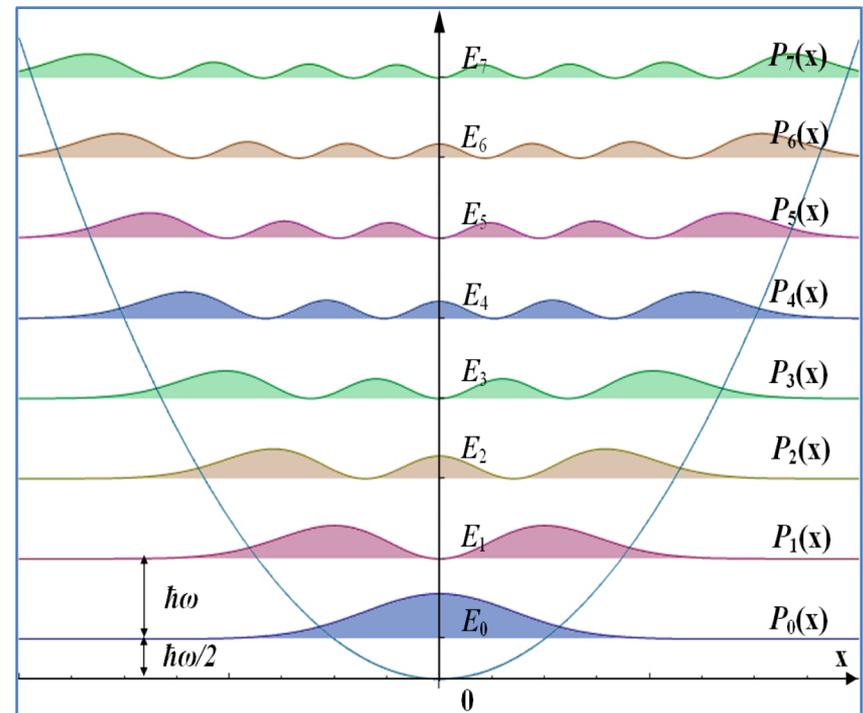
$$-\frac{1}{2} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi, \quad \text{with} \quad V(x) = \frac{1}{2}x^2$$

what is the natural scale for energy and length ?

- In dimensionless form the exact analytical eigenfunctions and the corresponding eigenvalues are

$$\psi_n(x) = \langle x | n \rangle = \frac{1}{\sqrt{2^n n!}} \pi^{-1/4} \exp(-x^2/2) H_n(x),$$

$$E_n = n + \frac{1}{2},$$



Practice Session #3

$$-\frac{1}{2} \frac{d^2 \psi}{dx^2} + V(x)\psi = E\psi, \quad \text{with} \quad V(x) = \frac{1}{2}x^2$$

1. Solve the equation in the domain $[-10,10]$ using $N = 800$ points, as initial condition the eigenfunction for the ground state $\exp(-x^2/2)$, its derivative and the exact eigenvalue ($E = 1/2$). Solve the equation forward (from $x=-10$ to $x=10$) and backwards (from $x=10$ to $x=-10$). What happens?
2. Now construct the residual by matching forward and backward numerical solutions at the matching point. Use the logarithmic derivative. Produce a plot with $0 < E < 5$. How many zero do you see?
3. Use bisection or false position to refine your search and converge to the eigenvalues.

Practice Session #3: Useful Tips

- Matching point: if $x_m=0$ is chosen to be the interval midpoint, then the logarithmic derivative may become ill-behaved due to the fact that the eigenfunctions of odd order have a zero. Therefore, it is advisable to use a point close to 0.
- Initial condition: to obtain a more accurate expression for the initial condition, one could use an asymptotic expansion of the original ODE. This can be rather complicated and outside this course objective; however we can obtain a simple expression by neglecting E:

$$\frac{d^2y}{dx^2} = x^2y \quad \rightarrow \quad y(x) = \sqrt{x} \left[c_1 I_{\frac{1}{4}} \left(\frac{x^2}{2} \right) + c_2 K_{\frac{1}{4}} \left(\frac{x^2}{2} \right) \right]$$

where $I_\nu()$ and $K_\nu()$ are the modified Bessel functions. The physical admissible solution is $K_\nu()$ and an asymptotic expansion for large x is

$$y(x) \sim \sqrt{\pi} e^{-\frac{x^2}{2}} \frac{1}{\sqrt{|x|}}$$

- Residual: a convenient way to normalize the residual is $\text{Res}(E) = \frac{A - B}{\sqrt{A^2 + B^2}}$
where $A=Y_L' Y_R$, $B=Y_R' Y_L$.

Homework

- Upload **qho.cpp**, with the three distinct sections (as explained previously) enclosed by preprocessor directives.
- In the file comment, at the beginning, report a table giving the number of iterations needed by the root solver to converge to the eigenvalue (stage #3). Write the table using a two-column format, where the 1st column is the eigenvalue computed numerically and the 2nd column is the corresponding number of iterations. Include at least 5 eigenvalues in increasing order.
- Use 14 intervals to bracket roots in the range $0 < E < 7$ when producing the table ($\text{eps} = 1.e-11$);