Lecture 7

Numerical Techniques: Differential Equations - Boundary Value Problems

Laplace Equation in Electrostatics

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Differential Equations

1 Initial Value Problems.

2 Boundary Value Problems:

The solution of the differential equation is searched within *certain constraints*, called the **boundary conditions**. For example,

$$\frac{d^2y}{dx^2} = f(x, y, y')$$

- If the solution of the equation in the interval of $x : [0, L]$ is required,
- the values at the y(0) and y(L) boundaries should be given.

3 Eigenvalue (characteristic-value) Problems.

Boundary/Eigen Value Problems I

- Consider a 2nd-order differential equation in the interval [a,b]:

$$y'' = f(x, y, y')$$

Two necessary conditions for the solution of this equation are given at two extremes:

$$\begin{aligned} y(a) &= A \\ y(b) &= B \end{aligned}$$

- This problem is more difficult to solve than the initial value problem that we previously discussed.
  - In initial value problem, $y(0)$ and $y'(0)$ are both given at $x = 0$.
  - It was possible to start with these two initial values and progress the solution through the interval.
  - In the boundary value problem, the number of initial conditions is insufficient.
- **We cannot directly obtain the solution with methods such as Euler or Runge-Kutta.**

Boundary/Eigen Value Problems II

- Eigenvalue problems are even more difficult.
- See the following 2nd degree differential equation:

$$y'' = f(x, y, y' : \lambda)$$

- Again, let the boundary conditions of this equation to be given at both ends.
- If these conditions can only be satisfied for *certain* λ *values*, we call it the *eigenvalue problem*.
  - e.g.: Vibrations of a wire with both ends fixed give stable solution only for *certain wavelengths*.
  - e.g.: Solutions of the Schrödinger equation that are zero at infinity exist only for *certain energy eigenvalues*.
- **In terms of numerical solution, boundary value and eigenvalue problems are solved by the same method.**

Linear Shooting I

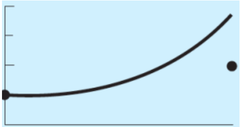

Figure: First guess.

Figure: Second guess.

. . .

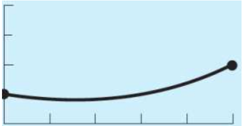

Figure: Expected result.

- The basic approach in solving **boundary value** and **eigenvalue problems** is known as the **trial-and-error method**.
  - At one boundary, the solution is started by giving an estimated value to the missing initial condition,
  - A trial solution is then found with either Euler or Runge-Kutta method at the other boundary (**First guess**),
  - How much deviation from the given boundary condition is determined,
  - Taking this deviation into account, a new solution is restarted with a new estimation (**Second guess**),
  - This process is repeated (. . .) until the other boundary condition is satisfied (**Expected result**).

Linear Shooting II

- Let's see this method on an example:

$$y''(x) - (4x^2 - 2)y = 0 \qquad \text{with BCs} \quad \begin{array}{l} y(0) = 1.0 \\ y(1) = 1/e = 0.36787944 \end{array}$$

- This differential equation has the solution of $y = e^{(-x^2)}$ (Gaussian function).

First, let's transform this boundary value problem into a first-order system of equations:

- $y_1 = y$
- $y_2 = y'$
- $\frac{dy_1}{dx} = y_2$
- $\frac{dy_2}{dx} = (4x^2 - 2)y_1$

- Notice that the boundary conditions are given only for y_1: $y_1(0) = 1.0$ and $y_1(1) = 0.368$.
- Notice that there is no initial condition for y_2.
- **Now, we have a set of equations.**

Linear Shooting III

- Here, let's take an estimated initial value of a:

$$\textbf{first guess}: \ y_2(0) = a$$

- Now, find the solutions $y_1(x)$ and $y_2(x)$ (by let's say RK4) with these $y_1(0)$ and $y_2(0)$ values.
- Denote the value obtained for y_1 in the other boundary with $y_{1a}(1)$
- and find the difference (Δ_a) with the real one $y_1(1)$ (here, 0.368):

$$y_2(0) = a \rightarrow solution: \ y_{1a}(x) \rightarrow \Delta_a = y_{1a}(1) - y_1(1)$$

- Now, let's make a **second (another) guess** of b and calculate the error again at the other boundary:

$$y_2(0) = b \rightarrow solution: \ y_{1b}(x) \rightarrow \Delta_b = y_{1b}(1) - y_1(1)$$

Linear Shooting IV

- Remind the secant methods for root finding.
- After these two estimated shoots, the most accurate starting value to choose will be the extension of the line passing through two points:

$$y_2(0) = b - \frac{\Delta_b}{\Delta_b - \Delta_a}(b - a)$$

- Then, the calculation (RK4) is repeated with this selected value by secant method.
- Finally, the solution is found when the margin of error in the other boundary is smaller than a certain tolerance.
- (**Example py-file:** mylinearshooting.py)

Linear Shooting V

```
Solution (y_2(0)) is found.
```

Step x	RK4 y	Exact y	RK4-Exact Error	SciPy y
0.00	1.0000000000000000	1.0000000000000000	0.0000000000000000	1.0000000000000000
0.01	0.9999000049788840	0.9999000049998333	0.0000000000209494	0.9999000049769683
0.02	0.9996000799477730	0.9996000799893344	0.0000000000415614	0.9996000797242913
0.03	0.9991004048166946	0.9991004048785274	0.0000000000618328	0.9991004045538127
0.04	0.9984012792358460	0.9984012793176064	0.0000000000817604	0.9984012793048143
0.05	0.9975031222961184	0.9975031223974601	0.0000000001013417	0.9975031227294181
0.06	0.9964064721104181	0.9964064722309933	0.0000000001205752	0.9964064724925857
0.07	0.9951119852763703	0.9951119854158298	0.0000000001394594	0.9951119851721190
0.08	0.9936204362211554	0.9936204363791490	0.0000000001579936	0.9936204356801045
0.09	0.9919327164293936	0.9919327166055711	0.0000000001761775	0.9919327149819753
0.10	0.9900498335551565	0.9900498337491681	0.0000000001940116	0.9900498322585485
0.90	0.4448580651753301	0.4448580662229407	0.0000000010476106	0.4448580640585380
0.91	0.4368785664741286	0.4368785675332217	0.0000000010590931	0.4368785643059327
0.92	0.4289563976083164	0.4289563986790725	0.0000000010707561	0.4289563954023433
0.93	0.4210936588053051	0.4210936598879114	0.0000000010826063	0.4210936573120806
0.94	0.4132923766756930	0.4132923777703437	0.0000000010946508	0.4132923758470025
0.95	0.4055545039564232	0.4055545050633201	0.0000000011068969	0.4055545032383834
0.96	0.3978819193318516	0.3978819204512042	0.0000000011193526	0.3978819180580180
0.97	0.3902764273314946	0.3902764284635206	0.0000000011320260	0.3902764252182211
0.98	0.3827397583031426	0.3827397594480686	0.0000000011449260	0.3827397559145742
0.99	0.3752735684599452	0.3752735696180068	0.0000000011580616	0.3752735662107565
1.00	0.3678794399999992	0.3678794411714418	0.0000000011714427	0.3678794377581407
1.01	0.3605588812968958	0.3605588824819751	0.0000000011850793	0.3605588789291024

Table: Solution for the Boundary Value Problem for the ODE: $y''(x) - (4x^2 - 2)y = 0$.

Linear Shooting VI

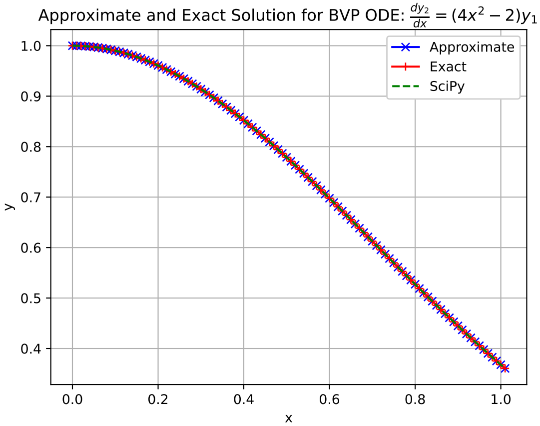

Figure: Solution for the Boundary Value Problem for the ODE: $y''(x) - (4x^2 - 2)y = 0$.

Laplace Equation in Electrostatics I

- The electrostatic potential created by a static charge distribution at a charge-free region is given by the following Laplace equation:

$$\nabla^2 V = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + + \frac{\partial^2 V}{\partial z^2} = 0$$

  Here, $V(x, y, z)$ is the potential within the region.
- The solution of this problem for particular charge distributions concerns the subject of **partial differential equations**.
- However, the dimensions of the problem can be reduced if the charge distribution exhibit a spatial symmetry.
- For example, in a system with **spherical symmetry**, the solution of the problem becomes easier if the partial derivatives in Laplace's equation are expressed in terms of **spherical coordinates** (r, θ, ϕ):

$$\nabla^2 V = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial V}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial V}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 V}{\partial \phi^2} = 0 \tag{1}$$

Laplace Equation in Electrostatics II

- Let the two concentric conductive spherical shells of radii R_a and R_b be held at constant potentials V_a and V_b (Figure).
- Because of spherical symmetry, the potential distribution in the region between the two spheres ($R_a < r < R_b$) will be a function of distance r only.
- Accordingly, the derivatives with respect to the variables (θ, ϕ) in Equation 1 become zero, and the partial derivative in the remaining term becomes the full derivative:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial V}{\partial r}\right) \rightarrow \frac{d^2 V}{dr^2} + \frac{2}{r}\frac{dV}{dr} = 0$$

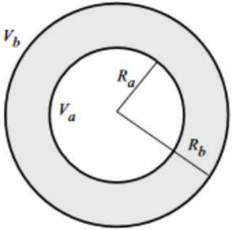

Figure: The region between two spherical shells of different potential.

The boundary conditions of this differential equation become:

$$V(R_a) = V_a$$
$$V(R_b) = V_b$$

Laplace Equation in Electrostatics III

As an example: Let's find the numerical solution of this equation for $R_a = 1\ m$, $R_b = 2\ m$, $V_a = 100\ V$, and $V_b = 0\ V$.

First, we transform this equation into a linear system of equations:

$$V \rightarrow V_1$$
$$\frac{dV}{dr} \rightarrow V_2$$

with these values ($V_1 and V_2$), the system of equations to be solved

$$\frac{dV_1}{dr} = V_2$$
$$\frac{dV_2}{dr} = -\frac{2}{r} V_2$$

and the boundary conditions are:

$$\begin{aligned} V(R_a) &= 100 \\ V(R_b) &= 0 \end{aligned}$$

- **Now, we have a set of equations.**
- The analytical solution to this spherically symmetric problem would be:

$$V(R) = \frac{R_a(R_b - r)}{(R_b - R_a)r} V_a$$

Laplace Equation in Electrostatics IV

We had a set of equations.
We transformed this boundary value problem into a first-order system of equations.

$$
\begin{aligned}
V_1 &= V \\
V_2 &= V' \\
\frac{dV_1}{dr} &= V_2 \\
\frac{dV_2}{dr} &= -\frac{2}{r} V_2
\end{aligned}
$$

(**Example py-file:** laplaceequation.py)

Laplace Equation in Electrostatics V

Solution (y_2(0)) is found.

Step x	RK4 y	Exact y	RK4-Exact Error	SciPy y
1.00	100.0000000000000000	100.0000000000000000	0.0000000000000000	100.0000000000000000
1.01	98.0198019839246939	98.0198019801980251	0.0000000037266688	98.0198019367090438
1.02	96.0784313796942087	96.0784313725490051	0.0000000071452035	96.0784311100688484
1.03	94.1747572918313125	94.1747572815533829	0.0000000102779296	94.1747572423479085
1.04	92.3076923208377877	92.3076923076923066	0.0000000131454811	92.3076924358639843
1.05	90.4761904919574107	90.4761904761904674	0.0000000157669433	90.4761904781525459
1.06	88.6792453011787103	88.6792452830188580	0.0000000181598523	88.6792450778453087
1.07	86.9158878708077509	86.9158878504672714	0.0000000203404795	86.9158877756185717
1.08	85.1851852075089937	85.1851851851851762	0.0000000223238175	85.1851853046562582
1.09	83.4862385562338716	83.4862385321100788	0.0000000241237927	83.4862385529654887
1.10	81.8181818439350366	81.8181818181817988	0.0000000257532378	81.8181816662801964
1.90	5.2631579000375517	5.2631578947367981	0.0000000053007536	5.2631578973265096
1.91	4.7120418895737144	4.7120418848167098	0.0000000047570046	4.7120419114658265
1.92	4.1666666708828348	4.1666666666666217	0.0000000042162132	4.1666667076922632
1.93	3.6269430088597163	3.6269430051813032	0.0000000036784131	3.6269430347455405
1.94	3.0927835082982367	3.0927835051545949	0.0000000031436418	3.0927835227867848
1.95	2.5641025667144475	2.5641025641025195	0.0000000026119280	2.5641025680749587
1.96	2.0408163286138654	2.0408163265305679	0.0000000020832975	2.0408163401195418
1.97	1.5228426411516396	1.5228426395938643	0.0000000015577752	1.5228426702649041
1.98	1.0101010111363471	1.0101010101009658	0.0000000010353813	1.0101010409498454
1.99	0.5025125633301593	0.5025125628140259	0.0000000005161334	0.5025125850668605
2.00	0.0000000000000022	-0.0000000000000444	0.0000000000000466	0.0000000206041846
2.01	-0.4975124383238556	-0.4975124378109786	0.0000000005128770	-0.4975124163493223

Table: Solution for the Boundary Value Problem for the ODE: $V'' = -\frac{2}{r} V'$.

Laplace Equation in Electrostatics VI

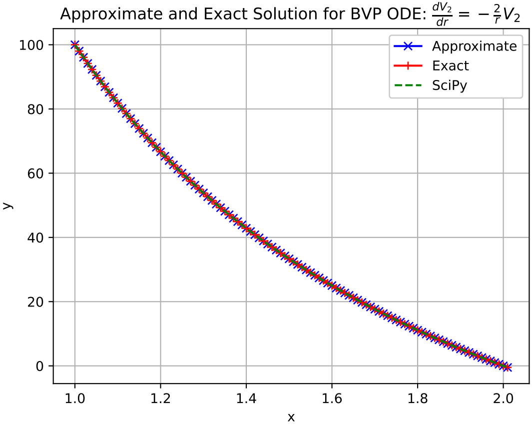

Figure: Solution for the Boundary Value Problem for the ODE: $V'' = -\frac{2}{r}V'$.