4.3 Boundary Value Problems

Examples:
- Poisson's and Laplace's equations,

$$d^2\phi/dx^2 = -\rho(x), \text{ or}$$

$$\begin{aligned} \frac{d\phi}{dx} &= -e \\ \frac{de}{dx} &= \rho(x) \end{aligned}$$

where $\rho(x)$ is a charge density. (Laplace: $\rho(x)=0$). Another physical problem described by the same equation is the temperature distribution along a thin rod: $d^2T/dx^2 = 0$.

- Time independent Schroedinger equation for a particle of mass m in a potential $U(x)$:

$$\frac{d^2\psi}{dx^2} = -g(x)\psi, \quad \text{with} \quad g(x) = \frac{2m}{\hbar^2}[E-U(x)]$$

The preceding physical examples belong to an important subclass of the general boundary value problem, in that they are all of the form $d^2y/dx^2 = -g(x)y + s(x)$. More generally, the 1-dimensional BVP reads

$$\frac{dy_i}{dx} = f_i(x, y_1, \dots y_N); \quad i = 1, \dots N$$

with N boundary values required. Typically there are

n_1 boundary values a_j $(j = 1, \dots n_1)$ at $x = x_1$, and
$n_2 \equiv N - n_1$ boundary values b_k $(k = 1, \dots n_2)$ at $x = x_2$.

The quantities y_i, a_j and b_k may simply be higher derivatives of a single solution function $y(x)$. Two methods are available, the *Shooting method* and the *Relaxation technique*.

Subsections

4.3.1 Shooting Method

- Transform the given *boundary* value problem into an *initial* value problem with estimated parameters

- Adjust the parameters iteratively to reproduce the given boundary values

First trial shot:

Augment the n_1 boundary values given at $x = x_1$ by $n_2 \equiv N - n_1$ *estimated* parameters

$$a^{(1)} \equiv \{a_k^{(1)};\ k = 1, \dots n_2\}^T$$

to obtain an IVP. Integrate numerically up to $x = x_2$. (For equations of the type $y'' = -g(x)y + s(x)$, Numerov's method is best.) The newly calculated values of b_k at $x = x_2$,

$$b^{(1)} \equiv \{b_k^{(1)};\ k = 1, \dots n_2\}^T$$

will in general deviate from the given boundary values $b \equiv \{b_k; \dots\}^T$. The difference vector $e^{(1)} \equiv b^{(1)} - b$ is stored for further use.

Second trial shot:

Change the estimated initial values a_k by some small amount, $a^{(2)} \equiv a^{(1)} + \delta a$, and once more integrate up to $x = x_2$. The values $b_k^{(2)}$ thus obtained are again different from the required values b_k: $e^{(2)} \equiv b^{(2)} - b$.

Quasi-linearization:

Assuming that the deviations $e^{(1)}$ and $e^{(2)}$ depend *linearly* on the estimated initial values $a^{(1)}$ and $a^{(2)}$, compute that vector $a^{(3)}$ which would make the deviations disappear:

$$a^{(3)} = a^{(1)} - A^{-1} \cdot e^{(1)}, \quad \text{with} \quad A_{ij} \equiv \frac{b_i^{(2)} - b_i^{(1)}}{a_j^{(2)} - a_j^{(1)}}$$

Iterate the procedure up to some desired accuracy.

EXAMPLE:

$$\frac{d^2y}{dx^2} = -\frac{1}{(1+y)^2} \quad \text{with} \quad y(0) = y(1) = 0$$

* *First trial shot:* Choose $a^{(1)} \equiv y'(0) = 1.0$. Applying 4th order RK with $\Delta x = 0.1$ we find $b^{(1)} \equiv y_{calc}(1) = 0.674$. Thus $e^{(1)} \equiv b^{(1)} - y(1) = 0.674$.

* *Second trial shot:* With $a^{(2)} = 1.1$ we find $b^{(2)} = 0.787$, i.e. $e^{(2)} = 0.787$.

* *Quasi-linearization:* From

$$a^{(3)} = a^{(1)} - \frac{a^{(2)} - a^{(1)}}{b^{(2)} - b^{(1)}} e^{(1)}$$

we find $a^{(3)} = 0.405(\equiv y'(0))$.

Iteration: The next few iterations yield the following values for $a(\equiv y'(0))$ and $b(\equiv y(1))$:

n	$a^{(n)}$	$b^{(n)}$
3	0.405	- 0.041
4	0.440	0.003
5	0.437	0.000

(Here ist the ANALYTICAL SOLUTION .)

4.3.2 Relaxation Method

Discretize x to transform a given DE into a set of algebraic equations. For example, applying DDST to

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

we find

$$\frac{d^2y}{dx^2} \approx \frac{1}{(\Delta x)^2}[y_{i+1} - 2y_i + y_{i-1}]$$

which leads to the set of equations

$$y_{i+1} - 2y_i + y_{i-1} - b_i(\Delta x)^2 = 0, \quad i = 2, \ldots M - 1$$

Since we have a BVP, y_1 and y_M will be given.

Let $y^{(1)} \equiv \{y_i\}$ be an inaccurate (estimated?) solution. The error components

$$e_i = y_{i+1} - 2y_i + y_{i-1} - b_i(\Delta x)^2, \quad i = 2, \dots M-1$$

together with $e_1 = e_M = 0$ then define an error vector $e^{(1)}$.

How to modify $y^{(1)}$ to make $e^{(1)}$ disappear? $\Longrightarrow$ Expand e_i linearly:

$$e_i(y_{i-1} + \Delta y_{i-1}, y_i + \Delta y_i, y_{i+1} + \Delta y_{i+1}) \approx e_i + \frac{\partial e_i}{\partial y_{i-1}} \Delta y_{i-1} + \frac{\partial e_i}{\partial y_i} \Delta y_i + \frac{\partial e_i}{\partial y_{i+1}} \Delta y_{i+1}$$

$$\equiv e_i + \alpha_i \Delta y_{i-1} + \beta_i \Delta y_i + \gamma_i \Delta y_{i+1} \quad (i = 1, \dots M)$$

This modified error vector is called $e^{(2)}$. We want it to vanish, $e^{(2)} = 0$:

$$A \cdot \Delta y = -e^{(1)} \quad \text{with} \quad A = \begin{pmatrix} 1 & 0 & 0 & \dots \\ \alpha_2 & \beta_2 & \gamma_2 & 0 \\ & \ddots & \ddots & \ddots \\ & & 0 & 1 \end{pmatrix}$$

Thus our system of equations is *tridiagonal*: $\Longrightarrow$ *Recursion technique!*

EXAMPLE:

$$\frac{d^2y}{dx^2} = -\frac{1}{(1+y)^2} \quad \text{with} \quad y(0) = y(1) = 0$$

DDST leads to $e_i = y_{i+1} - 2y_i + y_{i-1} + (\Delta x)^2/(1+y_i)^2$. Expand:

$$\alpha_i \equiv \frac{\partial e_i}{\partial y_{i-1}} = 1; \quad \gamma_i \equiv \frac{\partial e_i}{\partial y_{i+1}} = 1; \quad \beta_i \equiv \frac{\partial e_i}{\partial y_i} = -2\left[1 + \frac{(\Delta x)^2}{(1+y_i)^3}\right] \quad i = 2, \dots M-1$$

Start the downwards recursion: $g_{M-1} = -\alpha_M/\beta_M = 0$ and $h_{M-1} = -e_M/\beta_M = 0$.

$$g_{i-1} = \frac{-\alpha_i}{\beta_i + \gamma_i g_i} = \frac{-1}{\beta_i + g_i}; \quad h_{i-1} = \frac{-e_i - h_i}{\beta_i + g_i}$$

brings us down to g_1, h_1. Putting

$$\Delta y_1 = \frac{-e_1 - \gamma_1 h_1}{\beta_1 + \gamma_1 g_1} = e_1 (= 0)$$

we take the upwards recursion

$$\Delta y_{i+1} = g_i \Delta y_i + h_i; \quad i = 1, \dots M-1$$

Improve $y_i \longrightarrow y_i + \Delta y_i$ and iterate.

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