Computational Physics and Astrophysics

Ordinary Differential Equations
Boundary-value Problems

Kostas Kokkotas
University of Tübingen, Germany

and

Pablo Laguna
Georgia Institute of Technology, USA

Spring 2012

Ordinary Differential Equations

Consider a system of n ODEs

$$\vec{y}' = \vec{f}(x, \vec{y})$$

in the domain $[a, b]$ where $\vec{y} = (y_1, y_2, \ldots, y_n)$ and $\vec{f} = (f_1, f_2, \ldots, f_n)$.

- Recall that when solving this system as an initial value problem, all the conditions are specified at the same value of the independent variable on the equation. That is $\vec{y}(a) = \vec{y}_0$ or $\vec{y}(b) = \vec{y}_0$
- In a boundary-value problem, some of the conditions are specified at a and others at b.

Two-point Boundary Value Problem

Consider the following ODE,

$$\frac{d^2\phi}{dx^2} + u\,\frac{d\phi}{dx} + v\,\phi = \rho$$

where $x \in [a, b]$

Boundary Conditions

- Dirichlet: Specify the value of the solution. That is, $\phi(a) = \alpha$ and $\phi(b) = \beta$
- Neumann: Specify the value of the derivative. That is, $\phi'(a) = \alpha$ and $\phi'(b) = \beta$
- Mixed: using both Dirichlet and Neumann. That is, $\phi'(a) = \alpha$ and $\phi(b) = \beta$ or $\phi(a) = \alpha$ and $\phi'(b) = \beta$
- Robin:

$$\begin{aligned} c\,\phi(a) + d\,\phi'(a) &= g \\ e\,\phi(b) + f\,\phi'(b) &= h \end{aligned}$$

Approximate

$$\left.\frac{d^2\phi}{dx^2}\right|_i = \frac{\phi_{i+1} - 2\,\phi_i + \phi_{i-1}}{h^2}$$

$$\left.\frac{d\phi}{dx}\right|_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\,h}$$

Thus, in the interior points $i = 2, \cdots, N-1$ we have that

$$\frac{(\phi_{i+1} - 2\,\phi_i + \phi_{i-1})}{h^2} + u_i\,\frac{(\phi_{i+1} - \phi_{i-1})}{2\,h} + v_i\,\phi_i = \rho_i$$

Which can be re-written as

$$\left[\frac{1}{h^2} - \frac{u_i}{2\,h}\right]\phi_{i-1} + \left[v_i - \frac{2}{h^2}\right]\phi_i + \left[\frac{1}{h^2} + \frac{u_i}{2\,h}\right]\phi_{i+1} = \rho_i$$

This can be rewritten as

$$a_i\,\phi_{i-1} + b_i\,\phi_i + c_i\,\phi_{i+1} = d_i$$

where

$$\begin{aligned} a_i &= \left[\frac{1}{h^2} - \frac{u_i}{2\,h}\right] \\ b_i &= \left[v_i - \frac{2}{h^2}\right] \\ c_i &= \left[\frac{1}{h^2} + \frac{u_i}{2\,h}\right] \\ d_i &= \rho_i \end{aligned}$$

Tri-diagonal Matrix

The resulting system of algebraic equations has the following try-diagonal form

$$\begin{pmatrix} b_1 & c_1 & 0 & \dots & & & \\ a_2 & b_2 & c_2 & \dots & & & \\ 0 & a_3 & b_3 & \dots & & & \\ & & & \dots & & & \\ & & & \dots & b_{N-2} & c_{N-2} & 0 \\ & & & \dots & a_{N-1} & b_{N-1} & c_{N-1} \\ & & & \dots & 0 & a_N & b_N \end{pmatrix} \cdot \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \dots \\ \phi_{N-2} \\ \phi_{N-1} \\ \phi_N \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ \dots \\ d_{N-2} \\ d_{N-1} \\ d_N \end{pmatrix}$$

Method to Solve a Tri-diagonal System

$$a_i\, u_{i-1} + b_i\, u_i + c_i\, u_{i+1} = d_i$$

Forward substitution

$$\gamma_i = \begin{cases} \dfrac{c_i}{b_i} & i = 1 \\ \dfrac{c_{i-1}}{b_{i-1} - \gamma_{i-1}\, a_{i-1}} & i = 2, \ldots, n \end{cases}$$

$$u_i = \begin{cases} \dfrac{d_i}{b_i} & i = 1 \\ \dfrac{d_i - u_{i-1}\, a_i}{b_i - \gamma_i\, a_i} & i = 2, \ldots, n \end{cases}$$

Back substitution

$$u_i = u_i - \gamma_{i+1}\, u_{i+1} \qquad i = n-1, \ldots, 1$$

```
function u = tridiag(a,b,c,d,N);
% Numerical Recipes, Press et al.  1992

if (b(1)==0)
  fprintf(1,'Reorder equations')
  pause
end

gama = zeros(1:n);
beta = b(1);
u(1) = d(1)/beta;

% Decomposition and forward substitution
for j = 2:N
  gamma(j) = c(j-1)/beta;
  beta = b(j)-a(j)*gamma(j);
  if (beta==0)
    fprintf(1,'Solver failed...')
    pause
  end
  u(j) = (d(j)-a(j)*u(j-1))/beta;
end

% Perform the backsubstitution
for j = N-1:-1:1
  u(j) = u(j)-gamma(j+1)*u(j+1);
end

return;
```

Boundary Conditions Implementation

- Dirichlet: $\phi(a) = \alpha$ and $\phi(b) = \beta$ thus

$$a_1 = 0, \quad b_1 = 1, \quad c_1 = 0 \quad \text{and} \quad d_1 = \alpha$$

$$a_N = 0, \quad b_N = 1, \quad c_N = 0 \quad \text{and} \quad d_N = \beta$$

- Neumann: $\phi'(a) = \alpha$ and $\phi'(b) = \beta$

$$a_1 = 0, \quad b_1 = \frac{-1}{h}, \quad c_1 = \frac{1}{h} \quad \text{and} \quad d_1 = \alpha$$

$$a_N = \frac{-1}{h}, \quad b_N = \frac{1}{h}, \quad c_N = 0 \quad \text{and} \quad d_N = \beta$$

- Mixed: using both Dirichlet and Neumann. That is, $\phi'(a) = \alpha$ and $\phi(b) = \beta$ or $\phi(a) = \alpha$ and $\phi'(b) = \beta$
- Robin:

$$\begin{aligned} c\,\phi(a) + d\,\phi'(a) &= g \\ e\,\phi(b) + f\,\phi'(b) &= h \end{aligned}$$

General Two-Point Boundary Problems

Once again consider the following system of ODEs

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

with $x \in [a, b]$

At $x = a$

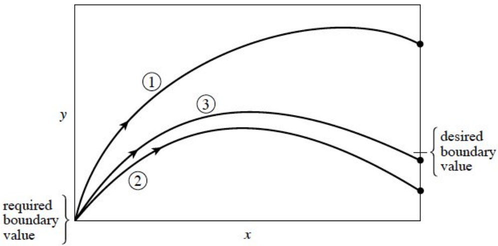
$$B_{1j}(a, y_1, \cdots, y_N) = 0 \quad i = 1, \cdots, n_1$$

At $x = b$

$$B_{2j}(b, y_1, \cdots, y_N) = 0 \quad i = 1, \cdots, n_2$$

such that $n_1 + n_2 = N$

Shooting Method



- At the starting point $x = a$ there are N starting values of y_i that need to be specified, but there are only n_1 conditions $B_{1j} = 0$.
- Thus, there are $n_2 = N - n_1$ freely specifiable starting values. Let's call those values $\vec{V} = (V_1, \cdots, V_{n_2})$.
- Therefore, with $B_{1j}\big|_{j=1,\cdots,n_1} = 0$ and $V_j\big|_{j=1,\cdots,n_2}$ we can contract the desired N starting values

$$y_i(a) = y_i(a, V_1, \cdots, V_{n_2}) \quad i = 1, \cdots, N$$

Shooting Method

- Given the values $y_i(a)$, one integrates the ODE to $x = b$ and obtains a set of N values $y_i(b)$.
- In general, these values will not satisfy the n_2 boundary conditions $B_{2j}(b, y_1, \cdots, y_N) = 0$
- Define the discrepancy vector $\vec{F}$ as

$$F_k = B_{2k}(b, y_1, \cdots, y_N) \quad k = 0, \cdots, n_2$$

- The goal is then given the free values $\vec{V}$ to shoot solutions until we get that $\vec{F} = 0$.
- That is, we are looking for the roots of $\vec{F}(\vec{V}) = 0$.
- One can use for instance bisection. We will try instead the Newton-Raphson method.

- The Newton-Raphson iterative procedure for this case is

$$\vec{F}(\vec{V}_{new}) = \vec{F}(\vec{V}_{old} + \delta\vec{V}) = \vec{F}(\vec{V}_{old}) + \overleftrightarrow{J} \cdot \delta\vec{V} = 0$$

with $\overleftrightarrow{J}$ the Jacobian matrix

$$J_{ij} = \frac{\partial F_i}{\partial V_j}$$

- Thus

$$\vec{V}_{new} = \vec{V}_{old} + \delta\vec{V}$$

in which $\delta\vec{V}$ is found from

$$\overleftrightarrow{J} \cdot \delta\vec{V} = -\vec{F}$$

- If the derivatives in the Jacobian are difficult to compute analytically, use instead

$$\frac{\partial F_i}{\partial V_j} \approx \frac{F_i(\cdots, V_j + \Delta V_j, \cdots) - F_i(\cdots, V_j, \cdots)}{\Delta V_j}$$

Shooting Method: Example

Consider the following ODE

$$\frac{d^2u}{dt^3} + u^2\frac{du}{dt} + u\cos(k\,t) = A\sin^2(q\,t)$$

with $t \in [a, b]$ and boundary conditions $u(a) = \alpha$, $u'(a) = 0$ and $u(b) = \beta$

Introduce the following definitions

$$\begin{aligned} y_1 &= u \\ y_2 &= \frac{du}{dt} \\ y_3 &= \frac{d^2u}{dt^2} \end{aligned}$$

Thus

$$\begin{aligned}
\frac{dy_1}{dt} &= y_2 \\
\frac{dy_2}{dt} &= y_3 \\
\frac{dy_3}{dt} &= -y_1^2\, y_2 - y_1\, \cos(k\, t) + A\, \sin^2(q\, t)
\end{aligned}$$

which has the desired form

$$\frac{dy_i(t)}{dt} = f_i(t, y_1, y_2, y_3) \quad i = 1, \cdots, 3$$

with boundary conditions

$$\begin{aligned}
y_1(a) &= \alpha \\
y_2(a) &= 0 \\
y_1(b) &= \beta
\end{aligned}$$

- To start integrating, we need a condition or guess for y_3; that is, $y_3(a) = V$
- This condition will yield a value y_1 at $x = b$ such that $y_1(b) - \beta = F \neq 0$
- The new guess for V is then obtained from

$$V_{n+1} = V_n + \delta V$$

$$\delta V = -\frac{F_n}{\left(\frac{dF}{dV}\right)_n}$$

$$\left(\frac{dF}{dV}\right)_n = \frac{F_n - F_{n-1}}{V_n - V_{n-1}}$$