Queens College, CUNY, Department of Computer Science

Numerical Methods

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Instructor: Dr. Sateesh Mane

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22 Lecture 22

Numerical solution of systems of ordinary differential equations

- In this lecture we study some simple examples of **boundary value problems**.
- We treat only second order (inhomogeneous) linear ordinary differential equations.
- Then the equation can be solved numerically using a tridiagonal matrix algorithm.

22.1 Basic equation

- The equation we shall solve in this lecture has the general form

$$\alpha(x)\,\frac{dy^2}{dx^2} + \beta(x)\,\frac{dy}{dx} + \gamma(x)y = \zeta(x)\,. \tag{22.1.1}$$

- Here $\alpha(x)$, $\beta(x)$, $\gamma(x)$ and $\zeta(x)$ are all functions of x only.
- We wish to solve for $y(x)$ in the interval $x_\ell \le x \le x_r$.
- Some of the values of $y(x)$ and/or dy/dx are given at the end point x_ℓ and others at the end point x_r.
- The above is called a **boundary value problem.**
- In this lecture, we require both x_ℓ and x_r to be finite.
- Our interest is to integrate eq. (22.1.1) numerically, using steps h_i, so $x_{i+1} = x_i + h_i$.
- We employ n subintervals, so end points are indexed as $x_0 = x_\ell$ and $x_n = x_r$.
- The steps h_i need not be of equal size, but in this lecture we shall assume equal steps $(= h)$.
- We define $y_i = y(x_i)$.

22.2 Finite differences: tridiagonal matrix equations

- The differential equation is given by eq. (22.1.1).
- We discretize the derivatives using centered finite differences.
- We employ uniform steps and n subintervals, hence $h = (x_r - x_\ell)/n$.
- Then the finite differences are

$$\frac{dy}{dx} = \frac{y_{i+1} - y_{i-1}}{2h}, \qquad \frac{d^2y}{dx^2} = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}. \tag{22.2.1}$$

- Substituting into eq. (22.1.1) yields the approximate numerical equation

$$\alpha(x_i)\,\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \beta(x_i)\,\frac{y_{i+1} - y_{i-1}}{2h} + \gamma(x_i)y_i = \zeta(x_i). \tag{22.2.2}$$

- Multiply through by h^2 and collect terms to obtain the following:

$$\begin{gathered} \alpha(x_i)\,(y_{i+1} - 2y_i + y_{i-1}) + \frac{h}{2}\beta(x_i)\,(y_{i+1} - y_{i-1}) + h^2\gamma(x_i)y_i = h^2\zeta(x_i) \\ \Big[\,\alpha(x_i) - \tfrac{1}{2}h\beta(x_i)\Big]\,y_{i-1} - \Big[\,2\alpha(x_i) - h^2\gamma(x_i)\Big]\,y_i + \Big[\,\alpha(x_i) + \tfrac{1}{2}h\beta(x_i)\Big]\,y_{i+1} = h^2\zeta(x_i). \end{gathered} \tag{22.2.3}$$

- Express eq. (22.2.3) in the form

$$b_i\,y_{i-1} + a_i\,y_i + c_i\,y_{i+1} = d_i\,, \tag{22.2.4a}$$
$$a_i = -2\alpha(x_i) + h^2\gamma(x_i)\,, \tag{22.2.4b}$$
$$b_i = \alpha(x_i) - \tfrac{1}{2}h\beta(x_i)\,, \tag{22.2.4c}$$
$$c_i = \alpha(x_i) + \tfrac{1}{2}h\beta(x_i)\,, \tag{22.2.4d}$$
$$d_i = h^2\zeta(x_i)\,. \tag{22.2.4e}$$

- Then eq. (22.2.4) yields a tridiagonal matrix system of equations (except at the end points). (Blanks denote zeroes in the tridiagonal matrix below.)

$$\begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ & b_{i-1} & a_{i-1} & c_{i-1} & & & \\ & & b_i & a_i & c_i & & \\ & & & b_{i+1} & a_{i+1} & c_{i+1} & \\ & & & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ y_{i-1} \\ y_i \\ y_{i+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ d_{i-1} \\ d_i \\ d_{i+1} \\ \vdots \end{pmatrix}. \tag{22.2.5}$$

- The boundary conditions will supply the equations to use at the end points $i = 0$ and $i = n$.
- **Note that in general, the tridigonal equations are NOT diagonally dominant.**

22.3 Tridiagonal matrix equations: boundary conditions

- Since eq. (22.1.1) is a second order linear differential equation, it requires two independent conditions to specify a unique solution.
- Since we are solving a boundary value problem, one condition must be specified at x_ℓ, i.e. $i = 0$ and the other at x_r, i.e. $i = n$.
- There are four cases: (i) y_0 is given, (ii) y_n is given, (iii) y'_0 is given, (iv) y'_n is given.
- **See next page(s).**

22.3.1 Value of y_0 is given. Boundary condition $y_0 = Y_\ell$.

- This case is easy.
- The first row (for $i = 0$) has $a_0 = 1$, $c_0 = 0$ and $d_0 = Y_\ell$
- The matrix looks like this:

$$\begin{pmatrix} 1 & 0 & 0 & \\ b_1 & a_1 & c_1 & \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \end{pmatrix} = \begin{pmatrix} Y_\ell \\ d_1 \\ \vdots \end{pmatrix} . \tag{22.3.1}$$

22.3.2 Value of y_n is given. Boundary condition $y_n = Y_r$.

- This case is easy.
- The last row (for $i = n$) has $a_n = 1$, $b_n = 0$ and $d_n = Y_r$
- The matrix looks like this:

$$\begin{pmatrix} \ddots & \ddots & \ddots & \\ & b_{n-1} & a_{n-1} & c_{n-1} \\ & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vdots \\ y_{n-1} \\ y_n \end{pmatrix} = \begin{pmatrix} \vdots \\ d_{n-1} \\ Y_r \end{pmatrix} . \tag{22.3.2}$$

22.3.3 Value of y'_0 is given. Boundary condition $y'_0 = Y'_\ell$.

- This case requires more work.
- For the first equation, we employ a forward finite difference and write

$$\begin{aligned} \frac{y_1 - y_0}{h} &= Y'_\ell\,, \\ y_1 - y_0 &= hY'_\ell\,. \end{aligned} \tag{22.3.3}$$

- The first row (for $i = 0$) has $a_0 = -1$, $b_0 = 1$ and $d_0 = hY'_\ell$
- The matrix looks like this:

$$\begin{pmatrix} -1 & 1 & 0 & \\ b_1 & a_1 & c_1 & \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \end{pmatrix} = \begin{pmatrix} hY'_\ell \\ d_1 \\ \vdots \end{pmatrix}\,. \tag{22.3.4}$$

- The forward derivative is a first order approximation.
- This reduces the overall accuracy of the numerical solution.

22.3.4 Value of y'_n is given. Boundary condition $y'_n = Y'_r$.

- This case requires more work.
- For the last equation, we employ a backward finite difference and write

$$\begin{aligned} \frac{y_n - y_{n-1}}{h} &= Y'_r\,, \\ y_n - y_{n-1} &= hY'_r\,. \end{aligned} \tag{22.3.5}$$

- The last row (for $i = n$) has $a_n = 1$, $b_n = -1$ and $d_0 = hY'_r$
- The matrix looks like this:

$$\begin{pmatrix} \ddots & \ddots & \ddots & \\ & b_{n-1} & a_{n-1} & c_{n-1} \\ & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} \vdots \\ y_{n-1} \\ y_n \end{pmatrix} = \begin{pmatrix} \vdots \\ d_{n-1} \\ hY'_r \end{pmatrix}. \tag{22.3.6}$$

- The backward derivative is a first order approximation.
- This reduces the overall accuracy of the numerical solution.

22.4 Example matrices

- We set $n = 4$ to keep the matrix size small.
- Example: values of y_0 and y_n are given.

$$\begin{pmatrix} 1 & 0 & & & \\ b_1 & a_1 & c_1 & & \\ & b_2 & a_2 & c_2 & \\ & & b_3 & a_3 & c_3 \\ & & & 0 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} Y_\ell \\ d_1 \\ d_2 \\ d_3 \\ Y_r \end{pmatrix} . \tag{22.4.1}$$

- Example: values of y'_0 and y_n are given.

$$\begin{pmatrix} -1 & 1 & & & \\ b_1 & a_1 & c_1 & & \\ & b_2 & a_2 & c_2 & \\ & & b_3 & a_3 & c_3 \\ & & & 0 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} hY'_\ell \\ d_1 \\ d_2 \\ d_3 \\ Y_r \end{pmatrix} . \tag{22.4.2}$$

- Example: values of y_0 and y'_n are given.

$$\begin{pmatrix} 1 & 0 & & & \\ b_1 & a_1 & c_1 & & \\ & b_2 & a_2 & c_2 & \\ & & b_3 & a_3 & c_3 \\ & & & -1 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} Y_\ell \\ d_1 \\ d_2 \\ d_3 \\ hY'_r \end{pmatrix} . \tag{22.4.3}$$

- Example: values of y'_0 and y'_n are given.

$$\begin{pmatrix} -1 & 1 & & & \\ b_1 & a_1 & c_1 & & \\ & b_2 & a_2 & c_2 & \\ & & b_3 & a_3 & c_3 \\ & & & -1 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} hY'_\ell \\ d_1 \\ d_2 \\ d_3 \\ hY'_r \end{pmatrix} . \tag{22.4.4}$$

22.5 Worked example

- Let us solve the following equation

$$x^2 \frac{d^2y}{dx^2} + 2x \frac{dy}{dx} + \nu y = e^x \,. \tag{22.5.1}$$

- Here ν is a constant. We set $\nu = 1.5$ in the numerical work below.

- The domain of integration is $-1 \le x \le 1$.

- We set $n = 1000$, hence $h = 2/1000 = 0.002$.

- From eq. (22.2.4), the tridiagonal equations are given by:

$$b_i \, y_{i-1} + a_i \, y_i + c_i \, y_{i+1} = d_i \,, \tag{22.5.2a}$$

$$a_i = -2x_i^2 + h^2\nu \,, \tag{22.5.2b}$$

$$b_i = x_i^2 - hx_i \,, \tag{22.5.2c}$$

$$c_i = x_i^2 + hx_i \,, \tag{22.5.2d}$$

$$d_i = h^2 \exp(x_i) \,. \tag{22.5.2e}$$

- For $h < x_i \le 1$, we see that $|b_i| = x_i^2 - hx_i$ and $|c_i| = x_i^2 + hx_i$.
  Also $|a_i| = 2x_i^2 - h^2\nu$ for $\nu = 1.5$. Then

$$\begin{aligned} |a_i| - (|b_i| + |c_i|) &= 2x_i^2 - h^2\nu - (x_i^2 - hx_i + x_i^2 + hx_i) \\ &= -h^2\nu \\ &< 0 \,. \end{aligned} \tag{22.5.3}$$

- Hence the equations are NOT diagonally dominant.

- Notice also that for $x \simeq 0$, the coefficients of both d^2y/dx^2 and dy/dx vanish, and the differential equation reduces to $\nu y \simeq 1$.

- *But the tridiagonal algorithm does not fail.*

- **See next page.**

22.5.1 Case 1: $y_0 = 0.75$, $y_n = 0.25$

- The equations are

$$\begin{pmatrix} 1 & 0 & & & \\ b_1 & a_1 & c_1 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{n-1} & a_{n-1} & c_{n-1} \\ & & & 0 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{n-1} \\ y_n \end{pmatrix} = \begin{pmatrix} 0.75 \\ h^2 \exp(x_1) \\ \vdots \\ h^2 \exp(x_{n-1}) \\ 0.25 \end{pmatrix} . \tag{22.5.4}$$

- The solution is plotted as the black curve in Fig. 1, for $\nu = 1.5$.

22.5.2 Case 2: $y'_0 = -1$, $y_n = 1$

- The equations are

$$\begin{pmatrix} -1 & 1 & & & \\ b_1 & a_1 & c_1 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{n-1} & a_{n-1} & c_{n-1} \\ & & & 0 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{n-1} \\ y_n \end{pmatrix} = \begin{pmatrix} -h \\ h^2 \exp(x_1) \\ \vdots \\ h^2 \exp(x_{n-1}) \\ 1 \end{pmatrix} . \tag{22.5.5}$$

- The solution is plotted as the red curve in Fig. 1, for $\nu = 1.5$.

22.5.3 Case 3: $y_0 = 1$, $y'_n = 1$

- The equations are

$$\begin{pmatrix} 1 & 0 & & & \\ b_1 & a_1 & c_1 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{n-1} & a_{n-1} & c_{n-1} \\ & & & -1 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{n-1} \\ y_n \end{pmatrix} = \begin{pmatrix} 1 \\ h^2 \exp(x_1) \\ \vdots \\ h^2 \exp(x_{n-1}) \\ h \end{pmatrix} . \tag{22.5.6}$$

- The solution is plotted as the blue curve in Fig. 1, for $\nu = 1.5$.

22.5.4 Case 4: $y'_0 = 0$, $y'_n = 0$

- The equations are

$$\begin{pmatrix} -1 & 1 & & & \\ b_1 & a_1 & c_1 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{n-1} & a_{n-1} & c_{n-1} \\ & & & -1 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{n-1} \\ y_n \end{pmatrix} = \begin{pmatrix} 0 \\ h^2 \exp(x_1) \\ \vdots \\ h^2 \exp(x_{n-1}) \\ 0 \end{pmatrix} . \tag{22.5.7}$$

- The solution is plotted as the green curve in Fig. 1, for $\nu = 1.5$.

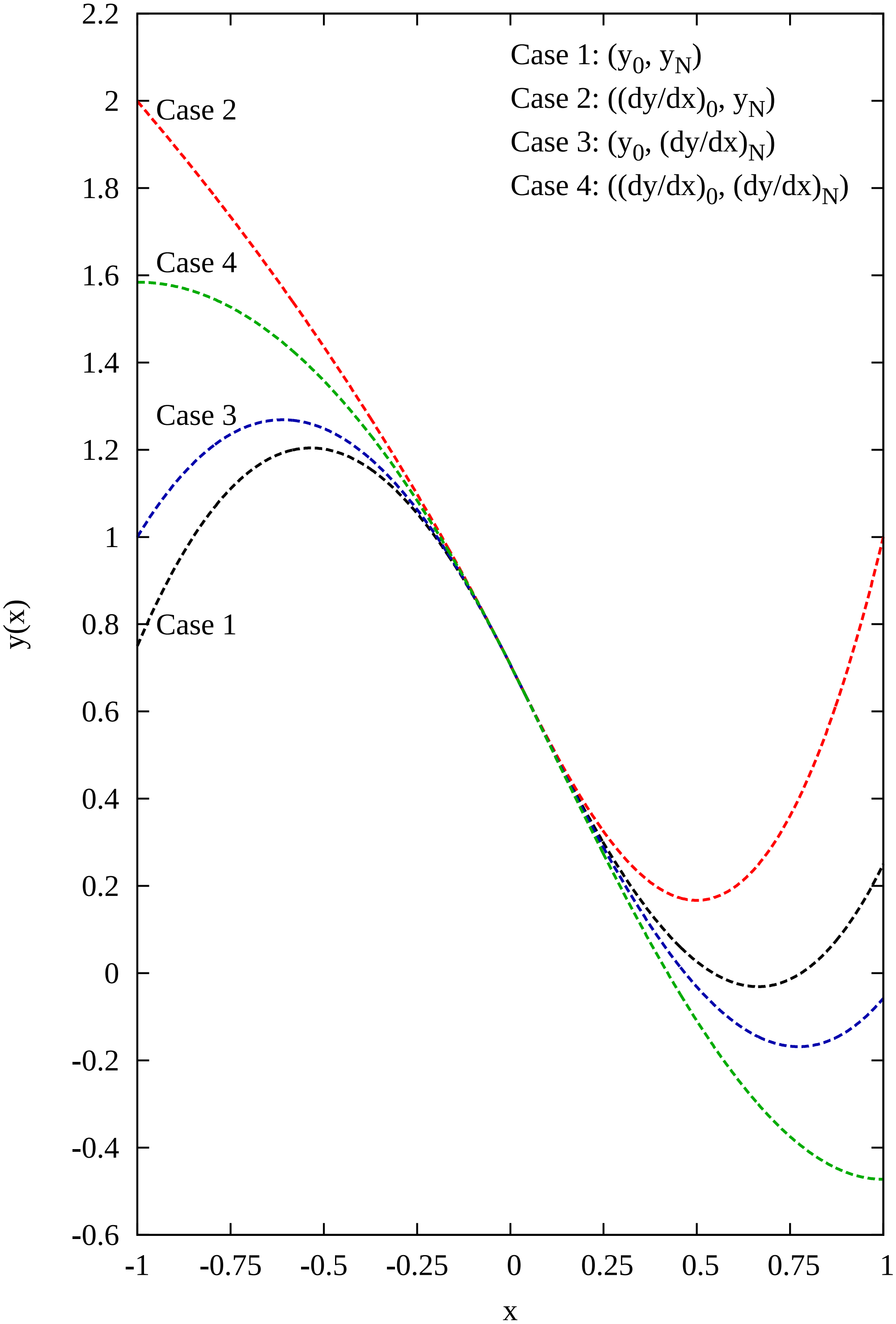

Figure 1: Solution of worked example in the text, for the four cases of boundary conditions: (i) (y_0, y_n), (ii) (y'_0, y_n), (iii) (y_0, y'_n) and (iv) (y'_0, y'_n).