Queens College, CUNY, Department of Computer Science

Numerical Methods

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17 Lecture 17

Numerical solution of systems of ordinary differential equations

- In this lecture we continue the study of initial value problems.
- This lecture is devoted to formal mathematical proofs.
- **The contents of this lecture are not for examination.**

17.1 Basic notation

- We repeat the basic definitions from the previous lecture.
- Let the system of coupled differential equations be

$$\frac{d\boldsymbol{y}}{dx} = \boldsymbol{f}(x, \boldsymbol{y})\,. \tag{17.1.1}$$

- There are n unknown variables y_j, $j = 1, \dots, n$.
- The starting point is $x = x_0$, and the initial value $\boldsymbol{y}_0$ is given.
- The above is called the **Cauchy problem** or **initial value problem.**
- Our interest is to integrate eq. (17.1.1) numerically, using steps h_i, so $x_{i+1} = x_i + h_i$.
- The steps h_i need not be of equal size.
- We define $\boldsymbol{y}_i = \boldsymbol{y}(x_i)$.

17.2 Trapezoid and midpoint methods

- The trapezoid and midpoint methods are both explicit second order numerical integration algorithms.
- Recall the formula for the trapezoid method:

$$\begin{aligned} \boldsymbol{g}_1 &= \boldsymbol{f}(x_i, \boldsymbol{y}_i)\,, && (17.2.1a)\\ \boldsymbol{g}_2 &= \boldsymbol{f}(x_i + h_i, \boldsymbol{y}_i + h_i\,\boldsymbol{g}_1)\,, && (17.2.1b)\\ \boldsymbol{y}_{i+1} &= \boldsymbol{y}_i + \frac{h_i}{2}\big(\boldsymbol{g}_1 + \boldsymbol{g}_2\big)\,. && (17.2.1c) \end{aligned}$$

- Recall the formula for the midpoiint method:

$$\begin{aligned} \boldsymbol{g}_1 &= \boldsymbol{f}(x_i, \boldsymbol{y}_i)\,, && (17.2.2a)\\ \boldsymbol{g}_2 &= \boldsymbol{f}\big(x_i + \tfrac{1}{2}h_i, \boldsymbol{y}_i + \tfrac{1}{2}h_i\,\boldsymbol{g}_1\big)\,, && (17.2.2b)\\ \boldsymbol{y}_{i+1} &= \boldsymbol{y}_i + h_i\,\boldsymbol{g}_2\,. && (17.2.2c) \end{aligned}$$

- Because the trapezoid and midpoint methods are **second order integration methods,** in both cases the numerical error in one integration step is of $O(h_i^3)$.
- In this lecture we shall give formal proofs that the numerical error in one integration step of the trapezoid and midpoint methods is of $O(h_i^3)$.

17.3 Derivation of numerical error of trapezoid method

- To keep the proof simple, we shall treat only the case of one unknown, which we shall call y.
- The differential equation is therefore

$$\frac{dy}{dx} = f(x,y)\,. \tag{17.3.1}$$

- Since we are analyzing only one integration step, we denote the stepsize by h.
- The formula for the trapezoid method is

$$y_{i+1} = y_i + \frac{h}{2}\Big[\,f(x_i,y_i) + f(x_i+h, y_i + hf(x_i,y_i))\Big]\,. \tag{17.3.2}$$

- The Taylor series for $y(x)$ is

$$y(x_i+h) = y(x_i) + h\,\frac{dy}{dx} + \frac{h^2}{2!}\,\frac{d^2y}{dx^2} + \frac{h^3}{3!}\,\frac{d^3y}{dx^3} + \cdots \tag{17.3.3}$$

- All the derivatives in eq. (17.3.3) are evaluated at $x = x_i$.
- Recall that for the explicit Euler method, we substituted for dy/dx to obtain

$$y(x_i+h) = y(x_i) + h\,f(x_i,y_i) + \frac{h^2}{2!}\,\frac{d^2y}{dx^2} + \cdots \tag{17.3.4}$$

- This was the proof that the error term for the explicit Euler method is $O(h^2)$, hence it is a first order method.
- We need to do more work to process the trapezoid method.
- We differentiate eq. (17.3.1) to obtain

$$\begin{aligned}\frac{d^2y}{dx^2} &= \frac{df(x,y)}{dx} \\ &= \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\,\frac{dy}{dx} \\ &= \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\,f\,.\end{aligned} \tag{17.3.5}$$

- For brevity, define a parameter k via

$$k = h\,f(x_i,y_i)\,. \tag{17.3.6}$$

- Next perform a two-dimensional Taylor series for $f(x_i+h, y_i+k)$ as follows. All the derivatives (and partial derivatives) are evaluated at (x_i, y_i). Then we obtain

$$
\begin{aligned}
f(x_i + h, y_i + k) &= f(x_i, y_i) + h\,\frac{\partial f}{\partial x} + k\,\frac{\partial f}{\partial y} \\
&\qquad + \frac{h^2}{2}\,\frac{\partial^2 f}{\partial x^2} + hk\,\frac{\partial^2 f}{\partial x \partial y} + \frac{k^2}{2}\,\frac{\partial^2 f}{\partial y^2} + \cdots \\
&= f(x_i, y_i) + h\,\frac{\partial f}{\partial x} + h\,\frac{\partial f}{\partial y}\,f \\
&\qquad + \frac{h^2}{2}\,\frac{\partial^2 f}{\partial x^2} + h^2\,\frac{\partial^2 f}{\partial x \partial y}\,f + \frac{h^2}{2}\,\frac{\partial^2 f}{\partial y^2}\,f^2 + \cdots
\end{aligned}
\tag{17.3.7}
$$

- Substituting in eq. (17.3.2) yields

$$
\begin{aligned}
y_{i+1} &= y_i + \frac{h}{2}\Big[\,f(x_i, y_i) + f(x_i + h, y_i + hf(x_i, y_i))\Big] \\
&= y(x_i) + \frac{h}{2}\Big[\,f(x_i, y_i) + f(x_i + h, y_i + k)\,\Big] \\
&= y(x_i) + h\,f(x_i, y_i) + \frac{h^2}{2}\left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\,f\right) + O(h^3) \\
&= y(x_i) + h\,\frac{dy}{dx} + \frac{h^2}{2}\,\frac{d^2 y}{dx^2} + O(h^3)\,.
\end{aligned}
\tag{17.3.8}
$$

- Hence the error term is of order $O(h^3)$ and the integration method is of second order.

17.4 Derivation of numerical error of midpoint method

- The proof is very similar to that for the trapezoid method in Sec. 17.3.
- Once again, we treat only the case of one unknown, which we shall call y.
- The differential equation is therefore given by eq. (17.3.1).
- We again denote the integration step by h.
- The formula for the midpoint method is

$$y_{i+1} = y_i + \frac{h}{2}\, f\big(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}hf(x_i, y_i)\big)\,. \tag{17.4.1}$$

- The Taylor series for $y(x)$ is given by eq. (17.3.3).
- Recall also

$$\frac{d^2y}{dx^2} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\, f\,. \tag{17.4.2}$$

- For brevity, define a parameter k via $k = h\, f(x_i, y_i)$.
- Next perform a two-dimensional Taylor series for $f\big(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k\big)$ as follows. All the derivatives (and partial derivatives) are evaluated at (x_i, y_i). Then we obtain

$$\begin{aligned}
f\big(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k\big) &= f(x_i, y_i) + \frac{h}{2}\frac{\partial f}{\partial x} + \frac{k}{2}\frac{\partial f}{\partial y} \\
&\qquad + \frac{h^2}{8}\frac{\partial^2 f}{\partial x^2} + \frac{hk}{4}\frac{\partial^2 f}{\partial x \partial y} + \frac{k^2}{8}\frac{\partial^2 f}{\partial y^2} + \cdots \\
&= f(x_i, y_i) + \frac{h}{2}\frac{\partial f}{\partial x} + \frac{h}{2}\frac{\partial f}{\partial y}\, f \\
&\qquad + \frac{h^2}{8}\frac{\partial^2 f}{\partial x^2} + \frac{h^2}{4}\frac{\partial^2 f}{\partial x \partial y}\, f + \frac{h^2}{8}\frac{\partial^2 f}{\partial y^2}\, f^2 + \cdots
\end{aligned} \tag{17.4.3}$$

- Substituting in eq. (17.4.1) yields

$$\begin{aligned}
y_{i+1} &= y_i + h\, f\big(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}hf(x_i, y_i)\big) \\
&= y(x_i) + h\, f\big(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k\big) \\
&= y(x_i) + h\, f(x_i, y_i) + \frac{h^2}{2}\left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\, f\right) + O(h^3) \\
&= y(x_i) + h\,\frac{dy}{dx} + \frac{h^2}{2}\frac{d^2y}{dx^2} + O(h^3)\,.
\end{aligned} \tag{17.4.4}$$

- Hence the error term is of order $O(h^3)$ and the integration method is of second order.

17.5 Lessons to learn

- There are various lessons to learn from the proofs in Secs. 17.3 and 17.4.
- In both cases, the proofs were based on Taylor series expansions.
- The above fact is significant.
  1. In both proofs we assumed that $y(x)$ is twice differentiable, i.e. that d^2y/dx^2 exists.
  2. This in turn assumes that $f(x, y)$ is differentiable in both x and y, i.e. that $\partial f/\partial x$ and $\partial f/\partial y$ both exist.
  3. In the case of $n > 1$ unknowns $y_1, \dots, y_n$ and n right-hand side functions $f_m(x, \boldsymbol{y})$, $m = 1, \dots, n$, we require the **Jacobian matrix** to exist. This is the matrix of the n^2 partial derivatives $\partial f_m/\partial y_j$, $1 \le j, m \le n$.
- However, it is possible that $\boldsymbol{y}(x)$ is *not* twice differentiable. It is possible that $\boldsymbol{f}$ is continuous but does not have well-defined partial derivatives for all n^2 entries in the Jacobian matrix.
- The proofs for higher order integration methods, such as fourth order Runge–Kutta `RK4`, are all based on Taylor series expansions.
- The higher the order of an integration method, the higher also the order of the partial derivatives of $\boldsymbol{f}$ which are required to exist, to justify the proof.
- This leads to the warning that **higher order does not always imply higher accuracy.**
- If $\boldsymbol{y}(x)$ is not twice differentiable, for example, a second (or higher) order integration method will not necessarily yield good results, or in any case it may not perform better than a first order integration method.
- The fourth order Runge–Kutta method `RK4` is widely used and is very popular. It is simple to code and works well in a wide variety of practical applications. Going beyond fourth order generally does not yield much additional benefit, relative to the extra computations involved.
- Hence most people do not employ integration methods beyond the fourth order.