Queens College, CUNY, Department of Computer Science

Numerical Methods

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15 Lecture 15

Numerical solution of systems of ordinary differential equations

- In this lecture we begin the study of **initial value problems**.
- These are systems of differential equations where the function values are specified at a starting point x_0 (or initial time t_0).
- The system of differential equations is then employed to propagate the solution forward.
- It is of course also possible to specify the function values at the end point (or final time), and to integrate the differential equations backwards.
  1. This is not necessarily a stupid thing to do.
  2. If we integrate a set of equations forward in time, it may be a good check to integrate them backwards to see if the solution returns to the original initial values.
  3. This can serve as a check on the numerical accuracy of the solution.
  4. Historically, this has been a valuable check on the accuracy of numerical integration algorithms.
  5. It also led to research on chaos in dynamical systems.
- The essential feature of an initial value problem is that all the function values are specified at one value of the independent variable x (or t).

15.1 Basic notation

- Let the system of coupled differential equations be

$$\frac{d\boldsymbol{y}}{dx} = \boldsymbol{f}(x, \boldsymbol{y}) \,. \tag{15.1.1}$$

- There are m unknown variables y_j, $j = 1, \dots, m$.
- 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. (15.1.1) 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 $\boldsymbol{y}_i = \boldsymbol{y}(x_i)$.

15.2 Euler integration

15.2.1 Explicit Euler method

- Let us employ a forward finite difference to approximate the derivative $d\boldsymbol{y}/dx$.
- Then we obtain the approximate finite difference equation

$$\frac{\boldsymbol{y}_{i+1} - \boldsymbol{y}_i}{h_i} \simeq \boldsymbol{f}(x_i, \boldsymbol{y}_i)\,. \tag{15.2.1}$$

- Rearranging terms yields the integration formula

$$\boldsymbol{y}_{i+1} = \boldsymbol{y}_i + h_i \boldsymbol{f}(x_i, \boldsymbol{y}_i)\,. \tag{15.2.2}$$

- The formula in eq. (15.2.2) is explicit, and is called the **explicit Euler method.**
- We obtain the numerical error estimate of the explicit Euler method by using a Taylor series

$$\boldsymbol{y}(x_i + h_i) = \boldsymbol{y}(x_i) + h_i \frac{d\boldsymbol{y}(x_i)}{dx} + \frac{h_i^2}{2} \frac{d^2\boldsymbol{y}(x_i)}{dx^2} + \dots \tag{15.2.3}$$

- Next substitute for $d\boldsymbol{y}/dx$ using eq. (15.1.1) to obtain

$$\boldsymbol{y}_{i+1} = \boldsymbol{y}_i + h_i\, \boldsymbol{f}(x_i, \boldsymbol{y}_i) + \boldsymbol{\frac{h_i^2}{2}\, y''(x_i)} + \dots \tag{15.2.4}$$

- The numerical error at the step i is of $O(h_i^2)$, hence eq. (15.2.2) is a **first order method.**
- For the variable y_j, $j = 1, \dots, m$, the magnitude of the error term ε_{ij} at the step i is

$$\varepsilon_{ij,\,\mathrm{exp}} = \frac{h_i^2}{2} |y_j''(x_i)|\,. \tag{15.2.5}$$

1. Obviously, eq. (15.2.5) assumes the function y_j is at least twice differentiable.
2. This need not be so in all problems.
3. In any case the error term is of order $O(h_i^2)$.

15.2.2 Implicit Euler method

- Let us employ a backward finite difference to approximate the derivative $d\boldsymbol{y}/dx$.
- Then we obtain the approximate finite difference equation

$$\frac{\boldsymbol{y}_{i+1} - \boldsymbol{y}_i}{h_i} \simeq \boldsymbol{f}(x_{i+1}, \boldsymbol{y}_{i+1})\,. \tag{15.2.1}$$

- Note that the right hand side is evaluated at x_{i+1}, not x_i.
- Rearranging terms yields the integration formula

$$\boldsymbol{y}_{i+1} - h_i \boldsymbol{f}(x_{i+1}, \boldsymbol{y}_{i+1}) = \boldsymbol{y}_i\,. \tag{15.2.2}$$

- The formula in eq. (15.2.2) is implicit, and is called the **implicit Euler method.**
  1. Because eq. (15.2.2) is an implicit equation, it must be solved for $\boldsymbol{y}_{i+1}$ via some (possibly nonlinear) root finding algorithm.
  2. The numerical solution of the implicit equation introduces an additional numerical error into the solution for $\boldsymbol{y}_{i+1}$.
  3. The numerical solution of the implicit equation also adds to the computation time of the algorithm.
- We obtain a numerical error estimate of the implicit Euler method by using a Taylor series

$$\boldsymbol{y}(x_{i+1} - h_i) = \boldsymbol{y}(x_{i+1}) - h_i\,\frac{d\boldsymbol{y}(x_{i+1})}{dx} + \frac{h_i^2}{2}\,\frac{d^2\boldsymbol{y}(x_{i+1})}{dx^2} + \dots \tag{15.2.3}$$

- Next substitute for $d\boldsymbol{y}/dx$ using eq. (15.1.1) to obtain

$$\boldsymbol{y}_{i+1} - h_i\,\boldsymbol{f}(x_{i+1}, \boldsymbol{y}_{i+1}) = \boldsymbol{y}_i - \boldsymbol{\frac{h_i^2}{2}\,y''(x_{i+1})} + \dots \tag{15.2.4}$$

- The numerical error at the step i is also of $O(h_i^2)$, hence eq. (15.2.2) is a **first order method.**
- However, note that because eq. (15.2.2) is an implicit formula, the above error analysis does not include the numerical error due to the approximation caused by the algorithm to solve the implicit equation.

15.2.3 Mixed explicit–implicit Euler method

- The mixed explicit–implicit Euler method yields the equation

$$\boldsymbol{y}_{i+1} - \frac{h_i}{2}\,\boldsymbol{f}(x_{i+1}, \boldsymbol{y}_{i+1}) = \boldsymbol{y}_i + \frac{h_i}{2}\,\boldsymbol{f}(x_i, \boldsymbol{y}_i) + \frac{h_i^2}{4}\,\big(\boldsymbol{y}''(x_i) - \boldsymbol{y}''(x_{i+1})\big) + \dots \tag{15.2.1}$$

- We might expect a partial cancellation, that $\boldsymbol{y}''(x_i) - \boldsymbol{y}''(x_{i+1}) = O(h)$, so that the mixed explicit–implicit Euler method yields a higher order algorithm.

- However, there are better ways to construct higher order integration algorithms.

15.2.4 Comments on the Euler method

- The Euler method is simple to understand and implement, but the numerical accuracy of the Euler method is usually too poor to be useful for practical applications.

- However, the basic ideas of the Euler method serve as the basis for the construction of better quality higher order integration algorithms.

15.3 Examples of Euler integration

- Let us consider the simple example equation (here c is a constant and $c > 0$)

$$\frac{dy}{dx} = -cy\,. \tag{15.3.1}$$

- The integration begins at $x_0 = 0$ and the initial value is $y_0 = 1$.
- The exact solution of eq. (15.3.1) is

$$y^{\rm ex}(x) = e^{-cx}\,. \tag{15.3.2}$$

- The above example was obviously chosen because we know the exact solution, hence we can compare the numerical solution to the exact answer.
- Let us integrate eq. (15.3.1) numerically using the explicit Euler method.

1. We employ a uniform stepsize h. Then $f(x_i, y_i) = -cy_i$ hence

$$y^{\rm exp}_{i+1} = y^{\rm exp}_i (1 - hc)\,. \tag{15.3.3}$$

2. The solution after n steps is

$$y^{\rm exp}_n = (1 - hc)^n\,. \tag{15.3.4}$$

3. Suppose we integrate out to a final value x_f and set $h = x_f/n$. Then we obtain

$$y^{\rm exp}(x_f) = \Bigl(1 - \frac{cx_f}{n}\Bigr)^n\,. \tag{15.3.5}$$

4. In the limit $n \to \infty$, i.e. $h \to 0$, the limit is e^{-cx_f}, which is the exact answer.

- Next us integrate eq. (15.3.1) numerically using the implicit Euler method.

1. We employ the same uniform stepsize h. Then $f(x_{i+1}, y_{i+1}) = -cy_{i+1}$. In this case the implicit equation solution can be solved easily and we obtain

$$\begin{aligned} y^{\rm imp}_{i+1} + hcy^{\rm imp}_{i+1} &= y^{\rm imp}_i \\ y^{\rm imp}_{i+1} &= \frac{y^{\rm imp}_i}{1 + hc}\,. \end{aligned} \tag{15.3.6}$$

2. The solution after n steps is

$$y^{\rm imp}_n = \frac{1}{(1 + hc)^n}\,. \tag{15.3.7}$$

3. Suppose we integrate out to a final value x_f and set $h = x_f/n$. Then we obtain

$$y^{\rm imp}(x_f) = \frac{1}{(1 + cx_f/n)^n}\,. \tag{15.3.8}$$

4. In the limit $n \to \infty$, i.e. $h \to 0$, the limit is $1/e^{cx_f}$ which also equals e^{-cx_f}.

15.4 Themes: why do we integrate?

- The two solutions in eqs. (15.3.4) and (15.3.7), and the other two solutions in eqs. (15.3.5) and (15.3.8) illustrate the two great themes of why we integrate to solve initial value problems.
- In eqs. (15.3.4) and (15.3.7), our basic mindset is to hold the stepsize h fixed and integrate for $n = 1, 2, 3, \ldots$ steps to see what happens.
- We wish to propagate the solution forwards, to **explore the unknown.**
  1. A typical physics problem might be to calculate the motion of a planet or comet or spacecraft, given the initial values for its position and velocity. We do not know where the object will travel and we wish to find out. Where will it go? What will it do?
  2. To answer such questions, we would like to have a high order integrator so that we can use a large stepsize h and still obtain results of good accuracy per step. Then we can integrate far out in space (or time) using only a small/moderate value of n.
- Conversely, in eqs. (15.3.5) and (15.3.8), our basic mindset is that the final location x_n is *fixed.* We wish to integrate from $x = x_0$ to x_f and obtain a solution of high accuracy at the final location x_f.
  1. We define $h = (x_f - x_0)/n$, so as the value of n increases, the value of h decreases, and the product nh remains fixed.
  2. For example, we have an optical system and we wish to form a high quality image on a screen. The length of the system (possibly a telescope or microscope or camera) is fixed.
  3. We are not integrating forwards to see where the system will travel at long distances. Instead we wish to obtain a highly accurate solution at a fixed target location x_f.
  4. We would like to have a high order integrator so that we can obtain good accuracy for the solution at x_f using only a relatively small value of n integration steps.
  5. In many cases, the high level task is a **design problem.**
     (a) For example, in an optical system, we may wish to design a beamline, to adjust the locations and strengths of lenses to form a good quality image on a final screen.
     (b) If we can get accurate results by integrating the differential equations using only a small value of n, then we can explore a large set of design scenarios.
     (c) An important goal is to find a design that achieves good results at minimal cost.
     (d) Correspondingly, if each integration is slow and requires a large value of n, we cannot test such a large set of design scenarios.
     (e) In my own work, I had to design a beamline for a particle accelerator. It was analogous to an optical system in many ways. The fundamental need was to be able to investigate a large variety of design scenarios. There was a need to an acceleator design that achieved good results at minimal cost. A fast integration algorithm was essential for the task.
- Hence in both cases, we wish to have a high order integrator, but for different reasons.

15.5 Graphs

- Let us plot some graphs for the case $c = 2$ in eq. (15.3.1).

  1. The exact solution of eq. (15.3.1) for $c = 2$ is $y^{\mathrm{ex}}(x) = e^{-2x}$.
  2. Let us set $h = 0.1$ and integrate from $x_0 = 0$ up to $x = 1$ in 10 steps, for both the explicit and implicit Euler methods.
  3. A graph of the exact answer and the numerical solution using the explicit Euler method is displayed in Fig. 1. The exact answer is plotted as the black curve and the numerical solution is plotted in red (with circles and lines).
  4. A graph of the exact answer and the numerical solution using the implicit Euler method is displayed in Fig. 2. The exact answer is plotted as the black curve and the numerical solution is plotted in red (with triangles and lines).

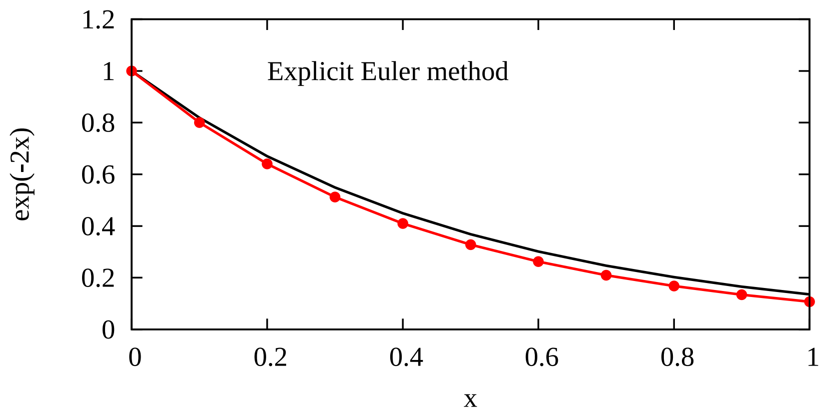

Figure 1: Graph of the solution of eq. (15.3.1) with plots of the exact solution $y = e^{-2x}$ (black) and the solution using the explicit Euler method (red), using eq. (15.3.3).

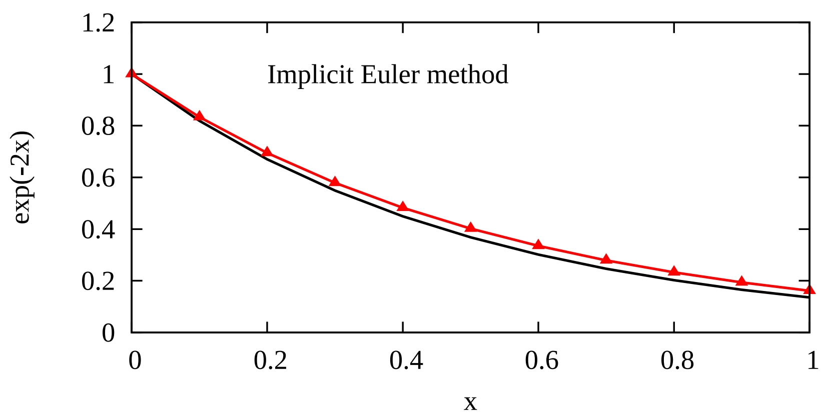

Figure 2: Graph of the solution of eq. (15.3.1) with plots of the exact solution $y = e^{-2x}$ (black) and the solution using the implicit Euler method (red), using eq. (15.3.6).

15.6 Simple error analysis I

- In the above example, with $c = 2$, the explicit Euler method underestimated the true answer in Fig. 1 and the implicit Euler method overestimated the true answer in Fig. 2.

- We can analyze the matter for arbitrary $c > 0$.

- For the exact solution, in one step we have, using $y^{\rm ex}(x) = e^{-cx}$,

$$y^{\rm ex}(x_i + h) = y^{\rm ex}(x_i)e^{-ch} \,. \tag{15.6.1}$$

- Let us begin with the explicit Euler method.

  1. We have seen that
  $$y^{\rm exp}(x_i + h) = y^{\rm exp}(x_i)(1 - ch) \,. \tag{15.6.2}$$
  2. It is a mathematical theorem that $e^{-ch} > 1 - ch$ for all real $h \neq 0$. Since the exact and numerical solution both begin with $y_0 = 1$, it follows that for all $x > 0$,
  $$y^{\rm exp}(x_i) < y^{\rm ex}(x_i) \,. \tag{15.6.3}$$

- Next let us analyze the implicit Euler method.

  1. We have seen that
  $$y^{\rm imp}(x_i + h) = \frac{y^{\rm imp}(x_i)}{1 + ch} \,. \tag{15.6.4}$$
  2. It is also a mathematical theorem that $e^{ch} > 1 + ch$ or equivalently $e^{-ch} < 1/(1 + ch)$ for all real $h \neq 0$. Since the exact and numerical solution both begin with $y_0 = 1$, it follows that for all $x > 0$,
  $$y^{\rm imp}(x_i) > y^{\rm ex}(x_i) \,. \tag{15.6.5}$$

- A better (or more relevant) analysis would treat the **local truncation error.**

- The **local truncation error** will be defined and discussed in future lectures.

15.7 Simple error analysis II: forward & backward integration

15.7.1 Explicit method

- Suppose we integrate forward for n steps and then reverse the direction and integrate backwards for n steps.
- Then we shall return to the starting value $x = x_0$ after $2n$ integration steps.
- The exact solution will return to its initial value y_0, ***but the numerical solution will not.***
- Let us use the previous example.
- Let us begin with the explicit Euler method.
- We saw that for one forward step

$$y_{i+1}^{\text{exp}} = y_i^{\text{exp}}(1 - ch)\,. \tag{15.7.1}$$

- Hence after n steps the solution is

$$y_n^{\text{exp}} = (1 - ch)^n\,. \tag{15.7.2}$$

- Now we reverse the direction of integration, i.e. replace h by $-h$.
- Then for one backward step we obtain

$$y_{i+1}^{\text{exp}} = y_i^{\text{exp}}(1 + ch)\,. \tag{15.7.3}$$

- Hence after $2n$ steps the solution is

$$y_{2n}^{\text{exp}} = (1 - ch)^n(1 + ch)^n = (1 - c^2h^2)^n\,. \tag{15.7.4}$$

- This is not equal to the initial value $y_0 = 1$.
- The difference is, assuming $c^2h^2 \ll 1$,

$$\begin{aligned} y_0 - y_{2n} &= 1 - (1 - c^2h^2)^n \\ &\simeq 1 - 1 + c^2h^2n \\ &= c^2h^2n\,. \end{aligned} \tag{15.7.5}$$

- If we employ a fixed stepsize h, then the error $|y_0 - y_{2n}|$ increases proportionally to n.
- If we integrate to a fixed final value $x = f_f$, then $h = (x_f - x_0)/n$ and then the difference is of order $1/n$:

$$y_0 - y_{2n} \simeq \frac{c^2(x_f - x_0)^2}{n}\,. \tag{15.7.6}$$

- These results are because the explicit Euler method is a first order integration algorithm.

15.7.2 Implicit method

- Next let us analyze the implicit Euler method.
- We saw that for one forward step

$$y_{i+1}^{\text{imp}} = \frac{y_i^{\text{exp}}}{1+ch}\,. \tag{15.7.1}$$

- Hence after n steps the solution is

$$y_n^{\text{imp}} = \frac{1}{(1+ch)^n}\,. \tag{15.7.2}$$

- Now we reverse the direction of integration, i.e. replace h by $-h$.
- Then for one backward step we obtain

$$y_{i+1}^{\text{imp}} = \frac{y_i^{\text{exp}}}{1-ch}\,. \tag{15.7.3}$$

- Hence after $2n$ steps the solution is

$$y_{2n}^{\text{imp}} = \frac{1}{(1-ch)^n(1+ch)^n} = \frac{1}{(1-c^2h^2)^n}\,. \tag{15.7.4}$$

- This is not equal to the initial value $y_0 = 1$.
- The difference is, assuming $c^2h^2 \ll 1$,

$$\begin{aligned} y_0 - y_{2n} &= 1 - \frac{1}{(1-c^2h^2)^n} \\ &\simeq 1 - 1 - c^2h^2n \\ &= -c^2h^2n\,. \end{aligned} \tag{15.7.5}$$

- If we employ a fixed stepsize h, then the error $|y_0 - y_{2n}|$ increases proportionally to n.
- If we integrate to a fixed final value $x = f_f$, then $h = (x_f - x_0)/n$ and then the difference is of order $1/n$:

$$y_0 - y_{2n} \simeq -\frac{c^2(x_f - x_0)^2}{n}\,. \tag{15.7.6}$$

- These results are because the explicit Euler method is a first order integration algorithm.

15.8 Simple stability analysis

- We know that for the problem in eq. (15.3.1) with $y_0 = 1$, the exact solution is $y^{\text{ex}}(x) = e^{-cx}$. Its value lies between 0 and 1 and decreases monotonically to zero as $x \to \infty$.

- For the explicit Euler method, from eq. (15.3.4) the solution after n steps is

$$y_n^{\text{exp}} = (1 - hc)^n \,. \tag{15.8.1}$$

  1. Suppose the value of c is large and the stepsize h is insufficiently small.
  2. Suppose in particular that $h > 1/c$. Then $1 - hc < 0$ and the explicit Euler method yields unphysical negative values.
  3. In fact, if $h > 2/c$, then $1 - hc < 0$ and $|1 - hc| > 1$. Then the solution $y^{\text{exp}}(x_i)$ alternates in sign as the value of i increases (unphysical) and also **the amplitude of the numerical solution grows to $+\infty$ as $x_i \to \infty$.**
  4. Both the negative values and the amplitude growth are wrong.
  5. If the stepsize is not small enough, the explicit Euler method can be unstable.

- For the implicit Euler method, from eq. (15.3.7) the solution after n steps is

$$y_n^{\text{imp}} = \frac{1}{(1 + hc)^n} \,. \tag{15.8.2}$$

  1. The denominator is always positive for all values of $h > 0$ (recall $c > 0$).
  2. The solution using the implicit Euler method always lies between 0 and 1 for $x > 0$, and decreases monotonically to zero as $x \to \infty$.
  3. If the value of h is not small enough, the solution from the implicit Euler method may not be very accurate, but ***it is stable*** and does not exhibit unphysical behavior such as negative values and/or amplitude growth.

- Although this is not a rigorously proved general statement, in many cases implicit integration algorithms have better stability (or a larger domain of stability) than explicit integration algorithms.

- For this reason, implicit integration algorithms continue to be employed in practical applications despite the computational complexity and cost of solving a set of implicit equations at each step.

- Of course, if we reverse the direction of integration, the implicit method yields

$$y_{2n}^{\text{imp}} = \frac{1}{(1 + hc)^n (1 - hc)^n} \,. \tag{15.8.3}$$

- Then if $hc = 1$ or $hc > 1$ the implicit Euler method is unstable and yields unphysical results.

- Hence the claims of “better stability” are not rigorously proved theorems for all situations.