0 Preliminaries

0.1 Motivation

The numerical methods of solving differential equations that we will study in this course are based on the following concept: Given a differential equation, e.g.,

$$y'(x) = f(x, y),$$
 (0.1)

replace the derivative by an appropriate *finite difference*, e.g.:

$$y'(x) \approx \frac{y(x+h) - y(x)}{h}$$
, when h is small $(h \ll 1)$. (0.2)

Then Eq. (0.1) becomes (in the approximate sense)

$$y(x+h) - y(x) = h f(x, y(x)),$$
(0.3)

from which the 'new' value y(x + h) of the unknown function y can be found given the 'old' value y(x).

In this course, we will consider both equations that are more complicated than (0.1) as well as the *discretization schemes* that are more sophisticated than (0.3).

0.2 Taylor series expansions

Taylor series expansion of functions will play a central role when we study the accuracy of discretization schemes. Below is a reminder from Calculus II, and its generalization.

If a function f(x) has infinitely many derivatives at $x = x_0$, then its Taylor series is:

$$f(x_0 + \Delta x) = f(x_0) + \frac{\Delta x}{1!} f'(x_0) + \frac{(\Delta x)^2}{2!} f''(x_0) + \dots$$

=
$$\sum_{n=0}^{\infty} \frac{(\Delta x)^n}{n!} f^{(n)}(x_0). \qquad (0.4)$$

If, however, f(x) is only known to have derivatives up to the (N + 1)st (i.e. $f^{(N+1)}(x_0)$ exists), then the following Taylor formula with a remainder holds:

$$f(x) = \sum_{n=0}^{N} \frac{(x-x_0)^n}{n!} f^{(n)}(x_0) + \frac{(x-x_0)^{N+1}}{(N+1)!} f^{(N+1)}(x^*), \quad \text{where } x^* \in (x_0, x) \,. \tag{0.5}$$

For functions of two variables, Eq. (0.4) generalizes as follows:

$$f(x_{0} + \Delta x, y_{0} + \Delta y) = \sum_{n=0}^{\infty} \frac{(\Delta x)^{n}}{n!} \frac{\partial^{n} f(x_{0}, y_{0} + \Delta y)}{\partial x^{n}}$$

$$= \sum_{n=0}^{\infty} \frac{(\Delta x)^{n}}{n!} \left(\sum_{m=0}^{\infty} \frac{(\Delta y)^{m}}{m!} \frac{\partial^{n+m} f(x_{0}, y_{0})}{\partial x^{n} \partial y^{m}} \right)$$

$$\stackrel{\text{explained below}}{=} \sum_{k=0}^{\infty} \frac{1}{k!} \left(\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y} \right)^{k} f(x, y)|_{x=x_{0}, y=y_{0}}$$

$$= f(x_{0}, y_{0}) + (\Delta x f_{x}(x_{0}, y_{0}) + \Delta y f_{y}(x_{0}, y_{0})) +$$

$$+ \frac{1}{2!} \left((\Delta x)^{2} f_{xx}(x_{0}, y_{0}) + 2\Delta x \Delta y f_{xy}(x_{0}, y_{0}) + (\Delta y)^{2} f_{yy}(x_{0}, y_{0}) \right) + \dots \quad (0.6)$$

The step of going from the second to the third line in the above calculations is based on the binomial expansion formula

$$(a+b)^{k} = \sum_{n=0}^{k} \frac{k!}{n!(k-n)!} a^{n} b^{k-n}$$

and takes some effort to verify. (For example, one would write out all terms in line two with n + m = 2 and verify that they equal to the term in line three with k = 2. Then one would repeat this for n + m = k = 3 and so on, until one sees the pattern.) For our purposes, it will be sufficient to just accept the end result, i.e. the last line of (0.6).

0.3 Existence and uniqueness theorem for ODEs

In the first two parts of this course, we will deal exclusively with ordinary differential equations (ODEs), i.e. equations that involve the derivative(s) with respect to only one independent variable (usually denoted as x).

To solve an ODE numerically, we first have to be sure that its solution exists and is unique; otherwise, we may be looking for something that simply is not there! The following theorem establishes this fundamental fact for ODEs.

Theorem 0.1 Let y(x) satisfy the initial-value problem (IVP), i.e. an ODE plus the initial condition:

$$y'(x) = f(x, y), \qquad y(x_0) = y_0.$$
 (0.7)

Let f(x, y) be defined and <u>continuous</u> in a closed region R that contains point (x_0, y_0) . Let, in addition, f(x, y) satisfy the *Lipschitz condition* with respect to y:

For any
$$x, y_1, y_2 \in R$$
, $|f(x, y_1) - f(x, y_2)| \le L|y_1 - y_2|$, (Lipschitz)

where the constant L depends on the region R and the function f, but not on y_1 and y_2 . Then a solution of IVP (0.7) exists and is unique on some interval containing the point x_0 .

<u>Remarks to Theorem 0.1</u>:

- 1. Any f(x, y) that is differentiable with respect to y and such that $|f_y| \leq L$ in R, satisfies the Lipschitz condition. In this case, the Lipschitz constant $L = \max_R |f_y(x, y)|$.
- 2. In addition, f(y) = |y| also satisfies the Lipchitz condition, even though this function does not have a derivative with respect to y. In general, $L = \max |f_y(x, y)|$, where the maximum is taken over the part of R where f_y exists. For example, for f(y) = |y|, one has L = 1.
- 3. $f(y) = \sqrt{y}$ does not satisfy the Lipschitz condition on [0, 1]. Indeed, one cannot find a constant L that would be independent of y and such that

$$\sqrt{y} - \sqrt{0} < L|y - 0|$$

for sufficiently small y.

Question: What happens to the solution of the ODE when the Lipschitz condition is violated?

Consider the IVP

$$y'(x) = \sqrt{y}, \qquad y(0) = 0.$$
 (0.8)

As we have just said in Remark 3, the function $f(y) = \sqrt{y}$ does not satisfy the Lipschitz condition. One can verify (by substitution) that IVP (0.8) has the following solutions:



Thus, if f(x, y) does not satisfy the Lipschitz condition, the solution of IVP (0.7) may not be unique.

If f(x, y) is a *linear* function of y, i.e.:

$$f(x,y) = a(x)y + g(x),$$
 (0.9)

then we have a stronger existence and uniqueness result than that given by Theorem 0.1. Namely, we have

Theorem 0.2 Let y(x) satisfy the linear IVP:

$$y'(x) = a(x)y + g(x), \qquad y(x_0) = y_0,$$
 (0.10)

where a(x) and g(x) are defined and continuous on an interval $(x_{\text{left}}, x_{\text{right}})$ that contains point x_0 . Then a solution of the IVP (0.10) exists, is unique, and has a continuous first derivative on the interval $(x_{\text{left}}, x_{\text{right}})$.

<u>Remarks to Theorem 0.2</u>:

1. The statement of Theorem 0.2 is stronger than that of Theorem 0.1 because the former guarantees a unique solution in the *entire* interval $(x_{\text{left}}, x_{\text{right}})$ where the coefficients of the ODE are defined. On the contrary, Theorem 1 guarantees a solution only on *some part*, but not necessarily all, of the interval where f(x, y) is defined as a function of x. Here is an example where the solution of an IVP fails to exist beyond some value of xeven though f(x, y) is defined for all x. Consider the IVP

$$y' = y^2, \qquad y(0) = 1.$$
 (0.11)

Here $f(x, y) = y^2$ is defined, continuous, and Lipshitz for all x and all finite y. However, the solution of (0.11), y = 1/(1-x), exists only on the interval [0, 1). It blows up at x = 1 and cannot be continued past that point.

Theorem 2 guarantees that such blow-ups or other "unpleasant" behavior will not occur for the linear IVP (0.10) with "well-behaved" coefficients a(x) and g(x). 2. The reason that makes the statement of Theorem 0.2 stronger than that of Theorem 0.1 is the fact that the right-hand side of (0.10) satisfies the Lipshitz condition for all y.

In contrast, $f(x, y) = y^2$ in the IVP (0.11) does not satisfy the Lipshitz condition when $y \to \infty$. Hence a blow-up, i.e. a behavior where $y \to \infty$, occurs for that IVP.

3. Coefficients a(x) and g(x) of the linear IVP (0.10) may have *finite* discontinuities. In such a case, the solution of the IVP will still exist and be unique, although it will have a discontinuous first derivative. You will encounter such a situation in Homework # 2.

0.4 Solution of a linear inhomogeneous IVP

Not only do we have the global existence and uniqueness result for the IVP (0.10), but we can also obtain the solution y(x) explicitly. Below we show how it can be done for a(x) = const.The general case is just slightly more technical, but conceptually similar.

Consider the IVP

$$y'(x) = a y + g(x), \qquad a = \text{const}, \qquad y(x_0) = y_0.$$
 (0.12)

Step 1: Solve the homogenous ODE y' = a y:

$$y'_{\text{hom}} = a y_{\text{hom}} \quad \Rightarrow \quad y_{\text{hom}}(x) = e^{a(x-x_0)}.$$
 (0.13)

Note that at this stage, $y_{\text{hom}}(x)$ is just *some* solution to the homogeneous ODE and does *not* need to satisfy the initial condition.

Step 2: Look for the solution of the inhomogeneous problem in the form $y(x) = y_{\text{hom}}(x) \cdot c(x)$, where c(x) is determined by substituting the latter expression into Eq. (0.12):

$$c y'_{\text{Mom}} + c' y_{\text{hom}} = a c y'_{\text{Mom}} + g(x), \qquad \Rightarrow$$

$$c' = \frac{g(x)}{y_{\text{hom}}}, \qquad \Rightarrow$$

$$c(x) = \int g(\bar{x}) e^{-a(\bar{x} - x_0)} d\bar{x}, \qquad \Rightarrow$$

$$y(x) = \left[y_0 + \int_{x_0}^x g(\bar{x}) e^{-a(\bar{x} - x_0)} d\bar{x} \right] e^{a(x - x_0)}. \qquad (0.14)$$

In the first line of (0.14), the symbol '/// ' denotes cancellation of the respective terms on the two sides of the equation, which occurs due to (0.13).

0.5 A very useful limit from Calculus

In Calculus I, you learned that

$$\lim_{h \to 0} (1+h)^{1/h} = e, (0.15)$$

where e is the base of the natural logarithm.

The following useful corollary is derived from (0.15):

$$\lim_{h \to 0} (1+ah)^{b/h} = e^{ab}, \tag{0.16}$$

where a, b are any finite numbers. Indeed, if we denote ah = g, then $g \to 0$ as $h \to 0$, and then the l.h.s. (left-hand side) of (0.16) becomes:

$$\lim_{g \to 0} (1+g)^{b/(g/a)} = \lim_{g \to 0} (1+g)^{ab/g} = \left(\lim_{g \to 0} (1+g)^{1/g}\right)^{ab} = e^{ab}.$$

Note also that

$$\lim_{h \to 0} (1 + ah^2)^{b/h} = e^0 = 1 \tag{0.17}$$

for any finite numbers a and b.