Integration and Differentiation

Numerical integration has been an active field in mathematics even before the introduction of computers since not all integrations can be carried out analytically and numerical methods become the only way to solve the problem. Furthermore, some common integrals have no analytical expression, such as the error function and gamma function. This is quite different from the differentiation. For most the smooth functions, differentiation can be carried out by analytical means. On some occasion, the functions for some physical quantities do not exist, and their derivatives can only be given numerically. Furthermore, numerical differentiation is a good way to be introduced to the wide world of finite difference methods for solving a large variety of problem, including differential equations.

3 Numerical integration

A standard one-dimensional definite integral with both upper and lower limits of the integration is represented by

$$I_{[a,b]} = \int_a^b f(x)dx.$$

The definition of the integral can be expressed in the following way. For simplicity we can assume that the integrand $f(x)$ is greater than or equal to zero everywhere in the interval $x = [a, b]$. Under such conditions the integral may be interpreted as the area bound above by $f(x)$, below by the x-axis, on the left by $x = a$ and on the right $x = b$. This form of integral is known in mathematics as the (definite) Riemann integral and is the only form with which we shall be dealing here.

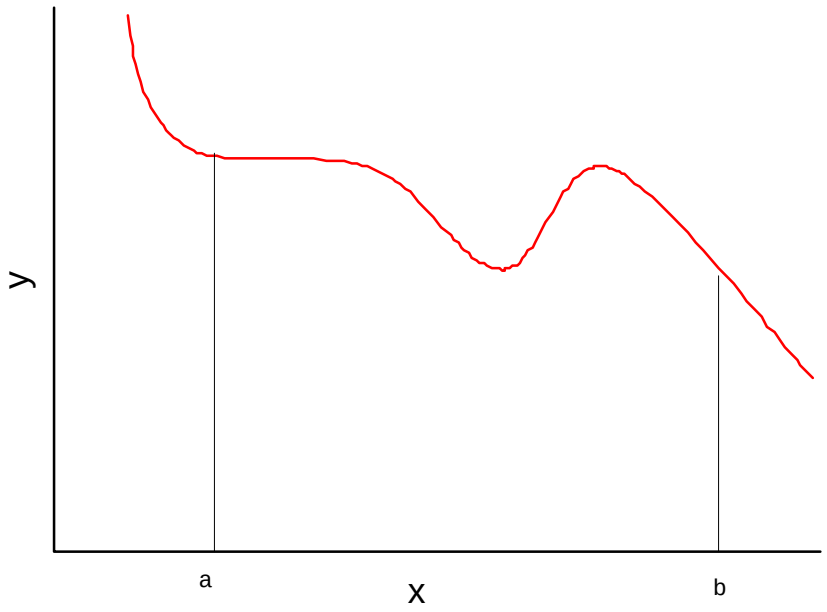

Figure 1:

The use of numerical integration may be illustrated using as an example the distance traveled by a particle moving along the x direction with velocity v. If v is a constant, the distance d covered in the integral between times $t = a$ and b is simply given by

$$d = v \times (b - a).$$

On the other hand, if the velocity varies as function of time, it is given, instead, by the integral

$$d = \int_a^b v(t)dt.$$

If $v(t)$ can be expressed in terms of some analytical function, the integral can usually be carried out without resorting to numerical methods. However, there are many occasions where $v(t)$ is available only as a table of data or in the form that cannot be integrated analytically.

Another example: a car travelling on a highway. If the only way we can find the velocity is to sample it once a minute, what is the distance travelled in, say, 10 minutes? In this case you have a set of data, NOT a smooth function. However we can get a very good estimate of the distance using the following approach. Since we do not know the exact velocity at all time we shall use the sampled result as the average velocity $\bar{v}$ (m/s) for that minute. The distance traveled in the minute is then $\bar{v} \times 10$ m. By summing all results in the ten minute, then we obtain the distance.

We divide the interval between $x = a$ and $x = b$ into a number of smaller one, say N subintervals. The width of the subinterval is

$$\begin{aligned} h &= (b-a)/N \\ &= x_i - x_{i-1}. \end{aligned}$$

The average of $f(x)$ in each subinterval is given by

$$\bar{f_i} = \frac{1}{h} \int_{x_{i-1}}^{x_i} f(x) dx.$$

Thus the integral can be defined as

$$I_{[a,b]} = \lim_{N \to +\infty} \frac{b-a}{N} \sum_{i=0}^{N} \bar{f_i}.$$

Actually this is the equivalent form of the original integral. The problem is how to calculate the average of $f(x)$ in each subintegral. Now the problem becomes how to calculate the average of $f(x)$ in each subintegral with finite N.

3.1 Rectangular rule

In practical calculation, it is impossible to take N infinite. We have to make some approximation by taking a finite N, and the error of the approximation also come from the approximation for the average of $f(x)$ in the subinterval. For the rectangular rule, the average of integrand in a subinterval is given by its value in the middle of the range,

$$\bar{f}_i = f(x_{i-1/2})$$

where $x_{i-1/2} = (x_{i-1} + x_i)/2$. To simplify the notation, we use

$$f_i \equiv f(x_i).$$

The integral is then

$$I_{[a,b]} = h \sum_{i=1}^{N} f_{i-1/2}.$$

Note that since we have taken $x_0 = a$, the estimate of $f(x)$ in the first interval $[a, a+h]$ is denoted as $f_{1/2} = f(x_{1/2})$. This method is known as the rectangular rule.

It is obvious that the average value of $f(x)$ in the subinterval $[x_i, x_{i+1}]$ is not exactly equal to the average value in the middle point of $[x_i, x_{i+1}]$. This is the main source of the error in the method. To check the accuracy of this approximation, we can expand the function $f(x)$ in terms of the Taylor series around the middle point $x_{i-1/2}$,

$$\begin{aligned} f(x) &= f_{i-1/2} + f'_{i-1/2}(x - x_{i-1/2}) \\ &\quad + \frac{1}{2!} f''_{i-1/2}(x - x_{i-1/2})^2 \\ &\quad + \frac{1}{3!} f'''_{i-1/2}(x - x_{i-1/2})^3 + \cdots \end{aligned}$$

The value of the integral in the subinterval may be expressed as

$$\begin{aligned}\int_{x_{i-1}}^{x_i} f(x)dx &= f_{i-1/2}\int_{x_{i-1}}^{x_i} dx \\ &+ f'_{i-1/2}\int_{x_{i-1}}^{x_i}(x-x_{i-1/2})dx \\ &+ \frac{1}{2!}f''_{i-1/2}\int_{x_{i-1}}^{x_i}(x-x_{i-1/2})^2dx \\ &+ \frac{1}{3!}f'''_{i-1/2}\int_{x_{i-1}}^{x_i}(x-x_{i-1/2})^3dx + \cdots\end{aligned}$$

In the integral the first term is the average value we used in the rectangular rule, and the second term vanishes. Therefore the leading error in the rectangular rule for the integral is given by

$$\triangle I_{[x_{i-1},x_i]} \equiv \int_{x_{i-1}}^{x_i} f(x)dx - hf_{i-1/2}$$

$$
\begin{aligned}
&\approx \frac{1}{2} f''_{i-1/2} \int_{x_{i-1}}^{x_i} (x - x_{i-1/2})^2 dx + \cdots \\
&\approx \frac{h^3}{24} f''_{i-1/2}
\end{aligned}
$$

The total error is

$$
\begin{aligned}
\triangle I_{[a,b]} &\equiv \int_a^b f(x)dx - I_{[a,b]} \\
&\approx \frac{(b-a)^3}{24N^2} f''(\xi)
\end{aligned}
$$

where $f''(\xi)$ is the average value of the second derivatives in $[a, b]$. Obviously $\triangle I_{[a,b]}$ becomes very small when N is large and $f(\xi)$ is a smooth function.

3.2 Trapezoidal rule

An alternative way to the rectangular rule is to approximate the area of each subinterval by a trapezoid instead of a rectangular by taking

$$\bar{f}_i = \frac{1}{2}(f_{i-1} + f_i).$$

For the entire interval $[a, b]$ the integral is given by the sum over all the slices,

$$\begin{aligned} I_{[a,b]} &= \frac{1}{2}h \sum_{i=1}^{N} (f_{i-1} + f_i) \\ &= h(\frac{1}{2}f_0 + f_1 + f_2 + \cdots + f_{N-1} + \frac{1}{2}f_N) \end{aligned}$$

This is a very reasonable result which we could have anticipated from the beginning. Compared with the others the contributions of f_0 and f_N are only half as important as they are located at the two ends of the interval.

The advantage of the trapezoidal rule is that the values of $f(x)$ are evaluated only on the grid or mesh points, that is at $x = x_0, x_1, \cdots, x_N$. The errors due to finite step sizes associated with this method are expected to be a factor of 2 larger than those of the rectangular rule.

3.3 Simpsom's rule

The errors associated with the rectangular and trapezoid rules are on the order of $1/N^2$. To improve the accuracy without increasing very much the amount of computation involved, we can use the Simpson's rule. We can take a Taylor series expansion of the area in two adjacent subintervals.

If the expansion is done around x_i the mid-point of the two subintervals combined, we obtain the result

$$\begin{aligned} I_{[x_{i-1},x_{i+1}]} &= \int_{x_{i-1}}^{x_{i+1}} f(x)dx \\ &= f_i \int_{x_{i-1}}^{x_{i+1}} dx + \frac{1}{1!} f_i' \int_{x_{i-1}}^{x_{i+1}} (x - x_i)dx \\ &\quad + \frac{1}{2!} f_i^{(2)} \int_{x_{i-1}}^{x_{i+1}} (x - x_i)^2 dx \\ &\quad + \frac{1}{3!} f_i^{(3)} \int_{x_{i-1}}^{x_{i+1}} (x - x_i)^3 dx \\ &\quad + \cdots \\ &= 2hf_i + 0 + \frac{1}{3} h^3 f_i^{(2)} + 0 + O(h^5 f_i^{(5)}). \end{aligned}$$

We see that the accuracy can be improved by two orders to $1/N^4$, if we can also include into the numerical integration terms involving the second order derivative of $f(x)$.

Using the central difference form the second-order derivative of $f(x)$,

$$\begin{aligned} f_i^{(2)} &= \frac{1}{h}\left[\frac{f_{i+1}-f_i}{h} - \frac{f_i - f_{i-1}}{h}\right] \\ &= \frac{1}{h^2}(f_{i+1} - 2f_i + f_{i-1}), \end{aligned}$$

the integral in the subinterval may be approximated as

$$I_{[x_{i-1},x_{i+1}]} = \frac{h}{3}(f_{i+1} + 4f_i + f_{i-1}) + O(h^5 f_i^{(5)}).$$

For the total value in the entire range,

$$\begin{aligned} I_{[a,b]} &= \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots \\ &\quad +2f_{N-2} + 4f_{N-1} + f_N) \end{aligned}$$

where N is an even number. In this way the accuracy of integration can be improved by two orders, $1/N^4$.

In addition to better accuracy, Simpson's rule has also the advantage that it leads naturally to a strategy for evaluating an integral to the desired accuracy by an iterative procedure. We start with $N = N_1$, where N_1 is some small but reasonable even number of interval. The integral can be divided into three parts,

$$\begin{aligned} S_d(N) &= f_0 + f_N \\ S_o(N) &= f_1 + f_3 + \cdots + f_{N-1} \\ S_e(N) &= f_2 + f_4 + \cdots + f_{N-2} \end{aligned}$$

and

$$I_{[a,b]}(N) = \frac{h}{3}[S_d(N) + 4S_0(N) + 2S_e(N)].$$

Next step is to double the number of subintervals by taking $N = N_2 = 2N_1$. The advantage of changing number of subintervals in this way is that, for the new N value, the contribution from the two end points, stored as

S_d, are unchanged, and the even grid points are exactly the ones already calculated in the previous iteration. The only new calculations required are the values of the function at the (new) odd grid points. Thus, we have

$$\begin{aligned} S_d(N_2) &= S_d(N_1) \\ S_e(N_2) &= S_e(N_1) + S_o(N_1) \\ S_o(N_2) &= \sum_{i=1}^{N_2/2} f(a + (2i-1)h) \end{aligned}$$

If the new result differs from the result in the previous iteration by an amount less than ϵ, the precision of the calculated value, we shall assume that the calculation have converged. Otherwise, we shall repeat to double the number of the subintervals until the convergence is reached. Since the leading error in this method is approximately proportional to $1/N^4$, in each iteration the precision of integral will increase by a factor, $1/2^4 = 1/16$.

Box 2-2 Program DM_SIMPS
Simpson's rule integration

Initialization:
- (a) Set ϵ as error tolerance and N as the initial number of points.
- (b) Set a maximum for the number of iterations allowed.

1. Input a as the lower limit of integration and b as the upper limit.
2. Make an initial calculation of the integral with N points:
   - (a) Calculate the contributions from end points.
   - (b) Sum over the contributions from odd points.
   - (c) Sum over the contributions from even points.
   - (d) Calculate the integral from these three terms using Eq. (2-16).
3. Double the number of points and calculate the value of the integral again:
   - (a) Sum the previous even and odd contributions as the new even value.
   - (b) Calculate the contribution from the new odd points.
   - (c) Calculate the integral with Eq. (2-16) using the new values.
4. Compare the new result with the previous one.
   - (a) If the difference is greater than ϵ go back to step 3.
   - (b) If the difference is smaller or equal to ϵ, return the result.

Figure 2:

3.4 Monte Carlo integration

For the discussion in this section, it is convenient to take the integration interval to be [0,1]. This choice is connected with the fact that most generators of random numbers with a uniform distribution are designed for this range. For integration with lower limit a different from zero, or upper limit b different from 1, it is a simple matter to make a transformation

$$x \rightarrow \frac{1}{b-a}(x-a)$$

so that the actual numerical integration is carried out in the interval [0, 1].

The Monte Carlo integration method is based on the idea that, instead of selecting the mesh points, we can take a random sample. If our sampling

is truly random, the points x_1, x_2, $\cdots$, x_N cover in the interval [0, 1] with equal probability. For N such points, the average distance between two adjacent ones is

$$h = \frac{1}{N-1} \to \frac{1}{N}.$$

The value of the integral is then

$$I_{[0,1]} = \int_0^1 f(x)dx \to \frac{1}{N}\sum_{i=1}^{N} f(x_i). \tag{1}$$

If our sampling is truly random, the number of points selected in a given region $[x - \Delta x/2, x + \Delta x/2]$ is independent of the value of x. In other words, if we divide the interval [0, 1] into an arbitrary number of equal size subintervals, the number of the points in each subinterval is the same within statistical fluctuations. Elementary notion of the statistics tells us that this can only be true if we take a large sample.

One difficulty inherent in Monte Carlo method is to know when N is large enough for Eq. 1 is valid. For our purpose here, we can take a practical approach and use an iterative strategy. We start with taking a sample of N_1 points and evaluate the integral in Eq. 1. The sampling is repeated for another N_1, and the integral is evaluated once again. If the two values are the same with some tolerance ε, it is likely that both samples are large enough. To improve the accuracy furthermore, we can combine the two samples and take the average of the two results. On the other hand if the difference is too large, we can take another sample of $2N_1$ points and evaluate the integral until the two results are the same within the ε.

$$
\begin{aligned}
I^{(1)}_{[0,1]}(N_1) &= \frac{1}{N_1}\sum_{i=1}^{N_1} f(x_i) \leftrightarrow I^{(2)}_{[0,1]}(N_1) = \frac{1}{N_1}\sum_{i=1}^{N_1} f(x_i) \\
I^{(1)}_{[0,1]}(2N_1) &= \frac{1}{2}\left[I^{(1)}_{[0,1]}(N_1) + I^{(2)}_{[0,1]}(N_1)\right]
\end{aligned}
$$

For multidimensional integrals, Monte Carlo methods may be more economical. Consider an example of a three dimensional integral:

$$I = \int_e^f \int_c^d \int_a^b f(x, y, z) dx dy dz.$$

Again, we can replace the integral by a sum over the products of values of the integral in each cell,

$$I \to \sum_{i=1}^{N} f(x_i, y_i, z_i) \triangle v$$

where

$$\triangle v = \frac{1}{N}(b - a)(d - c)(f - e).$$

Example: $I = \int_0^{\pi/2} \sin x dx$

Box 2-4 Program DM_MC1D
Monte Carlo integration for normal probability function

Subprogram used:
RSUB: Subtractive random number generator (Box 7-2)

Initialization:
(a) Set ϵ as the maximum error tolerated.
(b) Let N be the starting number of points for the integration.
(c) Zero the iteration counter and SUM.

1. Input:
   (a) Upper limit of the integral.
   (b) Seed for the random number generator.
2. Calculate the integral for N random points:
   (a) Generate a uniform random number t in $[0, 1]$.
   (b) Calculate the value of the integrand at t and add it to SUM.
3. Convert SUM to the value of the integral using Eqs. (2-34) and (2-35).
4. Repeat steps 2 and 3 with a different set of N random points.
5. Compare the two values of the integral obtained:
   (a) If the difference is larger than ϵ, then:
      (i) Take the average of the two values.
      (ii) Double the value of N.
      (iii) If less than the maximum number of iterations, go back to step 4.
      (iv) Otherwise return with error message.
   (b) If the difference is less than or equal to ϵ,
      Take the average of the two values and output the result.

Figure 3:

3.5 Improper integrals

In calculus, an improper integral is defined as one with either the range of integration being infinite or the integrand containing infinities within the integrand range. Obviously the singularities must be of a form that they do not make contributions such that the integral itself becomes infinite. For example,

$$I = \int_0^1 \frac{dx}{(1-x^2)^{1/2}}$$

has an singularity at the upper limit. However the integral itself exists and has the value $I = \pi/2$. On the other hand, the integral

$$I(y) = \int_0^y \frac{dx}{x}$$

does not exist (meaning, it does not have a finite value), since

$$\int \frac{dx}{x} = \ln x.$$

At the lower limit of 0, we have $\ln 0 \to -\infty$. We call the former type as an integrable singularity and the later one as a non-integrable singularity.

Example: $\sin x/x$

$$\frac{\sin x}{x} \to 1$$

as $x \to 0$. To avoid any overflow in the calculation, we put the condition that if $|x| < \epsilon$ let $\frac{\sin x}{x} \to 1$. The choice for the value of some small, positive number as the practical criterion such that the calculated value of integral is within the precision we want.

Example:

$$\int_0^{+\infty} e^{-x^2} dx = \frac{\pi}{2}.$$

We have a lot of methods to reduce the range of the integral to finite. For example,

$$\int_0^{+\infty} e^{-x^2} dx = \int_0^{b} e^{-x^2} dx + \int_b^{+\infty} e^{-x^2} dx$$

In this problem, the second term can be very samll for a large value of b because the value of the integrand is quite samll.

Let now turn our attention to integral containing integrable singularity inside the domain. Most of the numerical methods we have discussed so far may be used for this type integral, provided some minor modification are made to avoid the singular points. Since singularity cause overflows in the calculation, it is essential that they do not coincide with any of the

mesh points. For this reason, the Monte Carlo method is often the more convenient one to use improper integrals.

3.6 Example

3.6.1 Example 1 (from Numerical Recipes)

The program trapzd.c is applies the extended trapezoidal rule for integration. It is called sequentially for higher and higher stages of refinement of the integral. The sample xtrapzd uses trapzd to perform a numerical integration of the function

$$func = x^2(x^2 - 2)\sin x$$

whose indefinite integral is

$$\begin{aligned} fint &= \int dx x^2(x^2-2)\sin x \\ &= 4x(x^2-7)\sin x - (x^4-14x^2+28)\cos x. \end{aligned}$$

The integral is performed from $A = 0.0$ to $B = \pi/2$.

3.6.2 Example: Calculation of the period of pendulum

A pendulum is a system with mass m which is kept in orbit by a massless supporting rod of length l. The pendulum moves within the gravational field of the earth and is thus exposed to the vertical gravational force mg.

The dynamics force $\mathbf{F}$ is perpendicular to the supporting rod and takes the form

$$F = -mg \sin \phi.$$

For small amplitudes, we can model the pendulum in terms of a linear system which is equivalent to a harmonic oscillator. The accuracy of this approximation will be determined in the course of our calculation. The equation of motion can be derived from the equilibrium of the torque and product of angular acceleration and the momentum of inertia $I = ml^2$ with respect to the pivotal point:

$$\begin{aligned} I\frac{d^2\phi}{dt^2} &= lF. \\ \frac{d^2\phi}{dt^2} &= -\omega_0^2 \sin \phi \end{aligned}$$

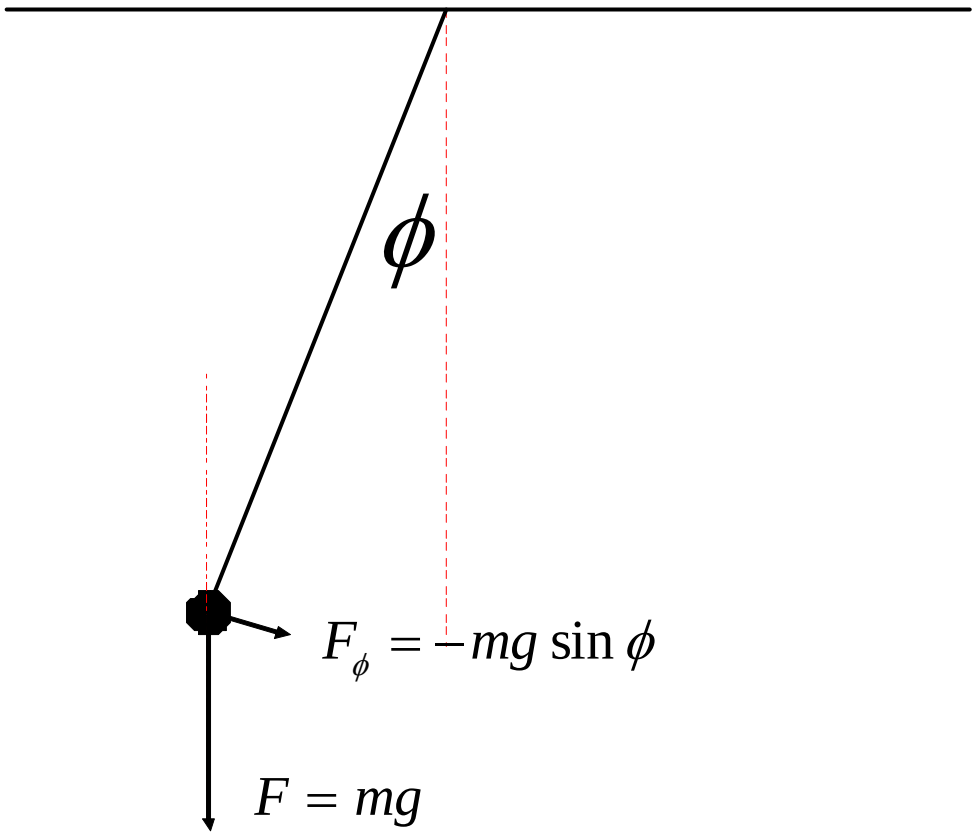

Figure 4:

where $\omega_0^2 = g/l$ being the ratio between the gravational acceleration g and the length of the pendulum l. The equation of motion can be solved numerically at this stage.

If the amplitude around the equilibrium position are small, $\sin\phi \approx \phi$. As a result, the equation of motion is reduced to an equation of simple harmonic oscillator,

$$\frac{d^2\phi}{dt^2} = -\omega_0^2\phi$$

Within this approximation the oscillation period T is given by

$$T = 2\pi/\omega_0.$$

Alternatively,

$$\frac{d^2\phi}{dt^2} = -\omega_0^2 \sin\phi$$

$$
\begin{aligned}
\frac{d}{dt}\dot{\phi}^2 &= 2\dot{\phi}\ddot{\phi} = -2\dot{\phi}\omega_0^2 \sin\phi \\
d\dot{\phi}^2 &= 2\dot{\phi}\ddot{\phi} = -2d\phi\omega_0^2 \sin\phi \\
\dot{\phi}^2 &= 4\omega_0^2(\sin^2\frac{\phi_0}{2} - \sin^2\frac{\phi}{2})
\end{aligned}
$$

Assuming $\dot{\phi} = 0$ at ϕ_0.

In general case, the total energy is conserved,

$$
\begin{aligned}
E &= T + V \\
&= \frac{1}{2}ml^2\dot{\phi}^2 + mgl(1 - \cos\phi) \\
&= mgl(1 - \cos\phi_0) \quad \text{(Initial condition)}
\end{aligned}
$$

We have an equation

$$
\dot{\phi}^2 = 4\omega_0^2(\sin^2\frac{\phi_0}{2} - \sin^2\frac{\phi}{2})
$$

and separation the variable, and we find

$$dt = \frac{1}{2\omega_0}(\sin^2\frac{\phi_0}{2} - \sin^2\frac{\phi}{2})^{-1/2}d\phi$$

Thus we can obtain the oscillation period T of the pendulum by integrating both sides over a complete period, the variable changes as $\phi_0 \to 0 \to -\phi_0 \to 0 \to \phi_0$,

$$T = \int_0^T dt = 4\int_0^{\phi_0} \frac{1}{2\omega_0}(\sin^2\frac{\phi_0}{2} - \sin^2\frac{\phi}{2})^{-1/2}d\phi.$$

$$T = \frac{2}{\omega_0}\int_0^{\phi_0}(\sin^2\frac{\phi_0}{2} - \sin^2\frac{\phi}{2})^{-1/2}d\phi.$$

The is a complete elliptic integral. You can do numerical integration at this step. To improve the efficiency, you may simplify the integral further. By substituting $z = \sin\frac{\phi}{2}/\sin\frac{\phi_0}{2}$ and $\alpha = \sin\frac{\phi_0}{2}$, the integral is transformed

to the standard form of

$$\begin{aligned} T &= \frac{4}{\omega_0}\int_0^1 \frac{dz}{(1-z^2)(1-\alpha^2 z^2)} \\ &= \frac{4}{\omega_0}K(\alpha^2). \end{aligned}$$

where $K(\alpha^2)$ denotes the complete elliptic integral of the first kind and $\alpha^2 = El/(2g)$.

Approximation:

$$\frac{1}{1-\alpha^2 z^2} = 1 + \frac{1}{2}\alpha^2 z^2 + \frac{3}{8}\alpha^4 z^4 + \cdots$$

3.7 PROBLEMS

1. Use a Monte Carlo method to carry out the integral

$$I = \int_0^1 \frac{dx}{1+x^2}$$

The result may be tested with the help of the relation

$$\int_0^1 \frac{da}{1+x^2} = \tan^{-1} x|_0^1 = \frac{\pi}{4}.$$

Is this a good way to obtain the value of π or just a way to test the random number generator used in the calculation?

2. Show that the error associated with the trapezoidal rule of integration for definite integral

$$I_{[a,b]} = \int_a^b f(x)dx$$

is $-(b-a)h^2 f''(\xi)/12$ where $f''(\xi)$ is the average value of the second order derivative of f(x) in the interval x=[a, b].

3. Compare the efficiencies of calculating the normal probability function integral

$$A(x) = \frac{1}{(2\pi)^{1/2}} \int_{-x}^{+x} e^{-t^2} dt$$

using the trapezoidal rule, Simpson's rule, and a Monte Carlo method.

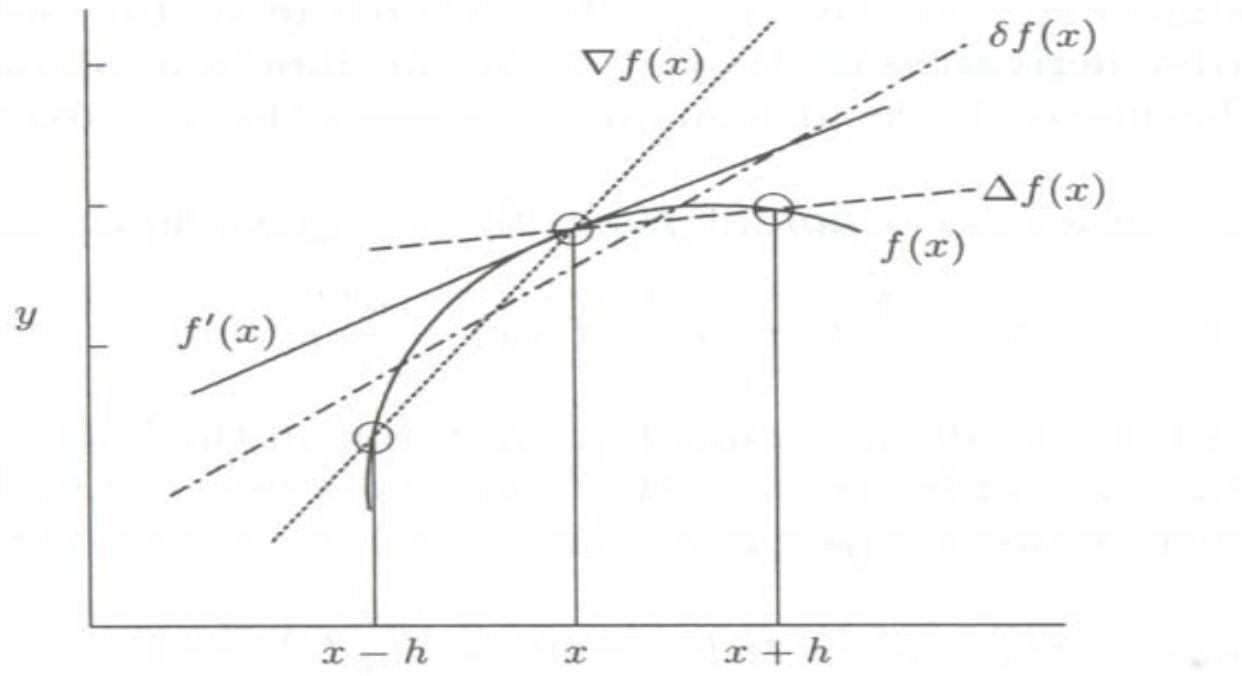

Figure 5: Schematic illustration of the various finite difference approximations to f'(x): dashed line, forward difference $\Delta f(x)$l dotted line, backward difference $\nabla f(x)$; dashed-dot line, central difference $\delta f(x)$; and exact value; solid line

4 Numerical differentiation

The first-order derivative of $f(x)$ is defined as

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

Graphically, we can think of $f'(x)$ as the slope or tangent, if $f'(x)$ at x. Since derivative of a function exist only as limiting values, it is impossible in numerical work to deal with them directly. Instead, we use finite difference, meaning small differences in the function near by points. There are several ways to define the finite difference:

The forward difference

$$\triangle f(x) = f(x+h) - f(x)$$

The backward difference

$$\nabla f(x) = f(x) - f(x - h)$$

The central difference

$$\delta f(x) = f(x + h/2) - f(x - h/2)$$

The most natural way to compute the first-order derivative for $f(x)$ at $x = x_i$ is to use the central difference,

$$f'(x) \approx \frac{\delta f(x)}{h}.$$

For many applications, the central difference is preferred over forward and backward difference. This is illustrated from the high order Taylor expan-

sion of $f(x \pm h)$ at x,

$$\begin{aligned} f(x \pm h) &= f(x) \pm h f'(x) + \frac{h^2}{2!} f''(x) \\ &\quad \pm \frac{h^3}{3!} f'''(x) + \cdots . \end{aligned}$$

This gives the result,

$$f'(x) = \frac{1}{h}(f(x+h) - f(x)) - \frac{h}{2} f''(x)$$

$$\begin{aligned} f'(x) &= \frac{1}{2h}\{f(x+h) - f(x-h)\} \\ &\quad - \frac{h^2}{3!} f'''(x) + \cdots \end{aligned}$$

The first term is identified to the central difference. The main error in the approximation come from the term with the order of h^2, which is smaller

by one order h than the forward and backward difference. Denote

$$x_k = x_0 + kh$$

The derivative can be taken as

$$\begin{aligned} f'_k &= \frac{f_{k+1} - f_{k-1}}{2k}; \\ f''_k &= \frac{f'_{k+1/2} - f'_{k-1/2}}{h} \\ &= \frac{f_{k+1} - 2f_k + f_{k-1}}{h^2} \end{aligned}$$

Using these results, we can make some improvement on the accuracy for derivatives in numerical calculation. For example,

$$\begin{aligned} f'_k &= \frac{1}{12h}(f_{k-2} - 8f_{k-1} + 8f_{k+1} - f_{k+2}) \\ &\quad + \frac{h^4}{30} f_k^{(5)} + \cdots \end{aligned}$$

Similarly, for the second order derivative,

$$\begin{aligned} f_k^{(2)} &= \frac{1}{12h^2}(-f_{k-2} + 16f_{k-1} \\ &\quad -30f_k + 16f_{k+1} - f_{k+2}) \\ &\quad + \frac{h^4}{90} f_k^{(6)} + \cdots . \end{aligned}$$

4.1 Example: $f(x) = e^{ikx}$

Consider the exponential function,

$$f(x) = e^{ikx}.$$

Analytically, the first-order derivative of the function is

$$f'(x) = ike^{ikx}.$$

To find the finite difference for $f(x)$, let us divide the abscissa x into equally spaced interval of width h each and as usual, use the symbol,

$$x_n = x_0 + nh$$

to represent the location of nth grid points from x_0 along the x-axis. Then the value of $f'(x)$ at x_n is

$$f'(x_n) = ike^{ikx_n}.$$

Forward difference:

$$f'(x_n) = \frac{f_{n+1} - f_n}{h} = ike^{ik(x_0+nh)}\frac{e^{ikh} - 1}{inh}.$$

Backward difference:

$$f'(x_n) = \frac{f_n - f_{n-1}}{h} = ike^{ik(x_0+nh)}\frac{1 - e^{-ikh}}{inh}.$$

Central difference:

$$f'(x_n) = \frac{f_{n+1} - f_{n-1}}{h} = ike^{ik(x_0+nh)}\frac{e^{ikh} - e^{-ikh}}{inh}.$$

To check the accuracy of various finite difference approximation, the results are

$$\frac{e^{ikh} - 1}{inh} = e^{ikh/2}\frac{\sin(kh/2)}{kh/2}$$

$$\frac{1 - e^{-ikh}}{inh} = e^{-ikh/2}\frac{\sin(kh/2)}{kh/2}$$

$$\frac{e^{ikh} - e^{-ikh}}{inh} = \frac{\sin(kh)}{kh}$$

For any finite size h, the absolute values are always less than unity unless $k = 0$. In other words, the numerical results constantly underestimate the derivative except for $k = 0$.

4.2 PROBLEM

Use a Taylor series expansion to derive the central difference result for the second-order derivative of $f(x)$ at $x = x_k$,

$$f''(x_k) = \frac{f_{k+1} - 2f_k + f_{k-1}}{h^2}.$$

Calculate the leading order correction term in powers of h.