Chapter 11

Finite Difference Approximation of Derivatives

11.1 Introduction

The standard definition of derivative in elementary calculus is the following

$$u'(x) = \lim_{\Delta x \to 0} \frac{u(x + \Delta x) - u(x)}{\Delta x} \tag{11.1}$$

Computers however cannot deal with the limit of $\Delta x \to 0$, and hence a *discrete* analogue of the continuous case need to be adopted. In a discretization step, the set of points on which the function is defined is finite, and the function value is available on a discrete set of points. Approximations to the derivative will have to come from this discrete table of the function.

Figure 11.1 shows the discrete set of points x_i where the function is known. We will use the notation $u_i = u(x_i)$ to denote the value of the function at the i-th node of the computational grid. The nodes divide the axis into a set of intervals of width $\Delta x_i = x_{i+1} - x_i$. When the grid spacing is fixed, i.e. all intervals are of equal size, we will refer to the grid spacing as Δx. There are definite advantages to a constant grid spacing as we will see later.

11.2 Finite Difference Approximation

The definition of the derivative in the continuum can be used to approximate the derivative in the discrete case:

$$u'(x_i) \approx \frac{u(x_i + \Delta x) - u(x_i)}{\Delta x} = \frac{u_{i+1} - u_i}{\Delta x} \tag{11.2}$$

where now Δx is finite and small but not necessarily infinitesimally small, i.e. . This is known as a *forward Euler* approximation since it uses forward differencing.

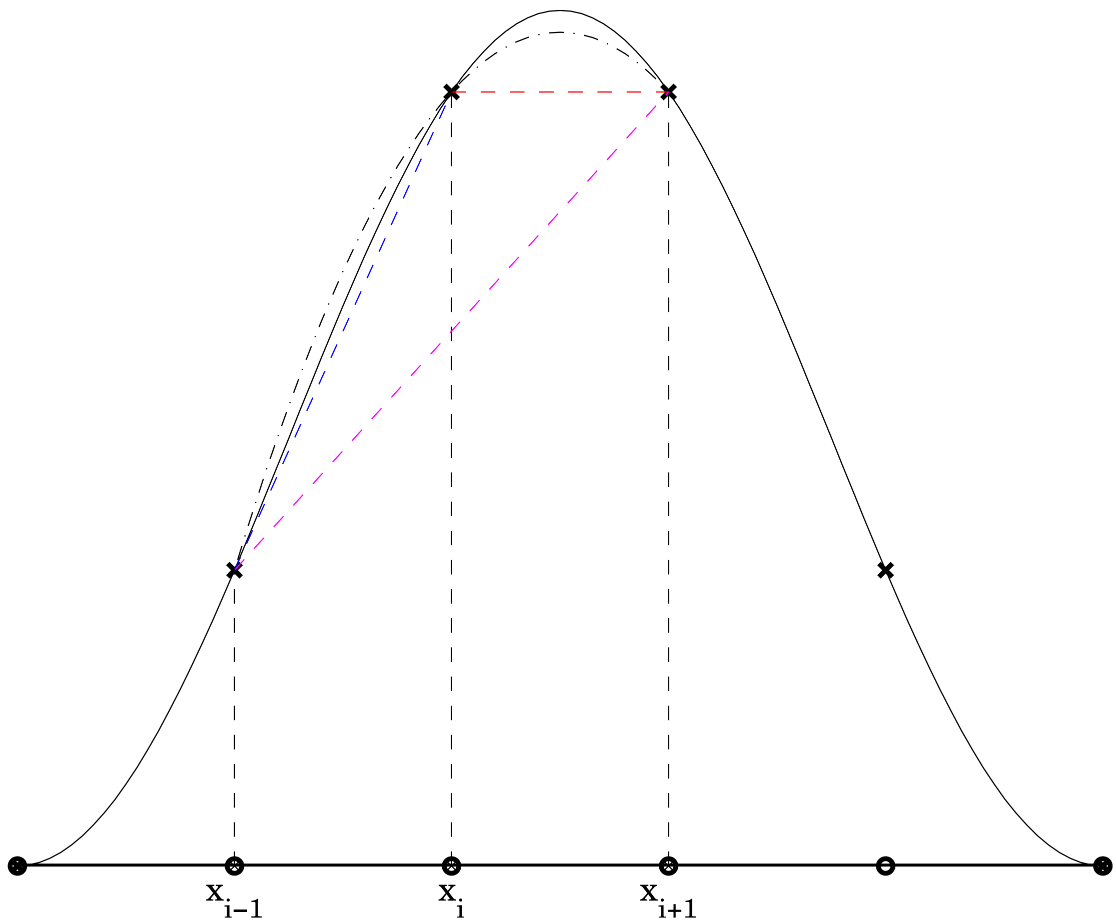

Figure 11.1: Computational grid and example of backward, forward, and central approximation to the derivative at point x_i. The dash-dot line shows the centered parabolic interpolation, while the dashed line show the backward (blue), forward (red) and centered (magenta) linear interpolation to the function.

Intuitively, the approximation will improve, i.e. the error will be smaller, as Δx is made smaller. The above is not the only approximation possible, two equally valid approximations are:
backward Euler:

$$u'(x_i) \approx \frac{u(x_i) - u(x_i - \Delta x)}{\Delta x} = \frac{u_i - u_{i-1}}{\Delta x} \tag{11.3}$$

Centered Difference

$$u'(x_i) \approx \frac{u(x_i + \Delta x) - u(x_i - \Delta x)}{2\Delta x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} \tag{11.4}$$

All these definitions are equivalent in the continuum but lead to different approximations in the discrete case. The question becomes which one is better, and is

there a way to quantify the error committed. The answer lies in the application of Taylor series analysis. We briefly describe Taylor series in the next section, before applying them to investigate the approximation errors of finite difference formulae.

11.3 Taylor series

Starting with the identity:

$$u(x) = u(x_i) + \int_{x_i}^{x} u'(s)\ \mathrm{d}s \tag{11.5}$$

Since $u(x)$ is arbitrary, the formula should hold with $u(x)$ replaced by $u'(x)$, i.e.,

$$u'(x) = u'(x_i) + \int_{x_i}^{x} u''(s)\ \mathrm{d}s \tag{11.6}$$

Replacing this expression in the original formula and carrying out the integration (since $u(x_i)$ is constant) we get:

$$u(x) = u(x_i) + (x - x_i)u'(x_i) + \int_{x_i}^{x}\int_{x_i}^{x} u''(s)\ \mathrm{d}s\ \mathrm{d}s \tag{11.7}$$

The process can be repeated with

$$u''(x) = u''(x_i) + \int_{x_i}^{x} u'''(s)\ \mathrm{d}s \tag{11.8}$$

to get:

$$u(x) = u(x_i) + (x - x_i)u'(x_i) + \frac{(x - x_i)^2}{2!}u''(x_i) + \int_{x_i}^{x}\int_{x_i}^{x}\int_{x_i}^{x} u'''(s)\ \mathrm{d}s\ \mathrm{d}s\ \mathrm{d}s \tag{11.9}$$

This process can be repeated under the assumption that $u(x)$ is sufficiently differentiable, and we find:

$$u(x) = u(x_i) + (x - x_i)u'(x_i) + \frac{(x - x_i)^2}{2!}u''(x_i) + \cdots + \frac{(x - x_i)^n}{n!}u^(n)(x_i) + R_{n+1} \tag{11.10}$$

where the remainder is given by:

$$R_{n+1} = \int_{x_i}^{x} \cdots \int_{x_i}^{x} u^{(n+1)}(x)(\ \mathrm{d}s)^{n+1} \tag{11.11}$$

Equation 11.10 is known as the Taylor series of the function $u(x)$ about the point x_i. Notice that the series is a polynomial in $(x - x_i)$ (the signed distance of x to x_i), and the coefficients are the (scaled) derivatives of the function *evaluated* at x_i.

If the $(n+1)$-th derivative of the function u has minimum m and maximum M over the interval $[x_i x]$ then we can write:

$$\int_{x_i}^{x} \cdots \int_{x_i}^{x} m(\,\mathrm{d}s)^{n+1} \le R_{n+1} \le \int_{x_i}^{x} \cdots \int_{x_i}^{x} M(\,\mathrm{d}s)^{n+1} \tag{11.12}$$

$$m\frac{(x-x_i)^{n+1}}{(n+1)!} \le R_{n+1} \le M\frac{(x-x_i)^{n+1}}{(n+1)!} \tag{11.13}$$

which shows that the remainder is bounded by the values of the derivative and the distance of the point x to the expansion point x_i raised to the power $(n+1)$. If we further assume that $u^{(n+1)}$ is continuous then it must take all values between m and M that is

$$R_{n+1} = u^{(n+1)}(\xi)\frac{(x-x_i)^{n+1}}{(n+1)!} \tag{11.14}$$

for some ξ in the interval $[x_i x]$.

11.3.1 Taylor series and finite differences

Taylor series have been widely used to study the behavior of numerical approximation to differential equations. Let us investigate the forward Euler with Taylor series. To do so, we expand the function u at x_{i+1} about the point x_i:

$$u(x_i + \Delta x_i) = u(x_i) + \Delta x_i \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x_i^2}{2!}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{\Delta x_i^3}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \ldots \tag{11.15}$$

The Taylor series can be rearranged to read as follows:

$$\frac{u(x_i + \Delta x_i) - u(x_i)}{\Delta x_i} - \left.\frac{\partial u}{\partial x}\right|_{x_i} = \underbrace{\frac{\Delta x_i}{2!}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{\Delta x_i^2}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \ldots}_{\text{Truncation Error}} \tag{11.16}$$

where it is now clear that the forward Euler formula (11.2) corresponds to truncating the Taylor series after the second term. The right hand side of equation (11.16) is the error committed in terminating the series and is referred to as the **truncation error**. The tuncation error can be defined as the difference between the partial derivative and its finite difference representation. For sufficiently smooth functions, i.e. ones that possess continuous higher order derivatives, and sufficiently small Δx_i, the first term in the series can be used to characterize the order of magnitude of the error. The first term in the truncation error is the product of the second derivative evaluated at x_i and the grid spacing Δx_i: the former is a property of the function itself while the latter is a numerical parameter which can be changed. Thus, for finite $\frac{\partial^2 u}{\partial x^2}$, the numerical approximation depends lineraly on the parameter Δx_i. If we were to half Δx_i we ought to expect a linear decrease

in the error for sufficiently small Δx_i. We will use the "big Oh" notation to refer to this behavior so that T.E. $\sim O(\Delta x_i)$. In general if Δx_i is not constant we pick a representative value of the grid spacing, either the average of the largest grid spacing. Note that in general the exact truncation error is not known, and all we can do is characterize the behavior of the error as $\Delta x \rightarrow 0$. So now we can write:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_i}{\Delta x_i} + O(\Delta x) \tag{11.17}$$

The taylor series expansion can be used to get an expression for the truncation error of the backward difference formula:

$$u(x_i - \Delta x_{i-1}) = u(x_i) - \Delta x_{i-1} \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x_{i-1}^2}{2!} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} - \frac{\Delta x_{i-1}^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{11.18}$$

where $\Delta x_{i-1} = x_i - x_{i-1}$. We can now get an expression for the error corresponding to backward difference approximation of the first derivative:

$$\frac{u(x_i) - u(x_i - \Delta x_{i-1})}{\Delta x_{i-1}} - \left.\frac{\partial u}{\partial x}\right|_{x_i} = \underbrace{-\frac{\Delta x_{i-1}}{2!} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{\Delta x_{i-1}^2}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots}_{\text{Truncation Error}} \tag{11.19}$$

It is now clear that the truncation error of the backward difference, while not the same as the forward difference, behave similarly in terms of order of magnitude analysis, and is linear in Δx:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_i - u_{i-1}}{\Delta x_i} + O(\Delta x) \tag{11.20}$$

Notice that in both cases we have used the information provided at just two points to derive the approximation, and the error behaves linearly in both instances.

Higher order approximation of the first derivative can be obtained by combining the two Taylor series equation (11.15) and (11.18). Notice first that the high order derivatives of the function u are all evaluated at the same point x_i, and are the same in both expansions. We can now form a linear combination of the equations whereby the leading error term is made to vanish. In the present case this can be done by inspection of equations (11.16) and (11.19). Multiplying the first by Δx_{i-1} and the second by Δx_i and adding both equations we get:

$$\frac{1}{\Delta x_i + \Delta x_{i-1}} \left[\Delta x_{i-1} \frac{u_{i+1} - u_i}{\Delta x_i} + \Delta x_i \frac{u_i - u_{i-1}}{\Delta x_{i-1}} \right] - \left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{\Delta x_{i-1} \Delta x_i}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{11.21}$$

There are several points to note about the preceding expression. First the approximation uses information about the functions u at three points: x_{i-1}, x_i and x_{i+1}.

Second the truncation error is T.E. $\sim O(\Delta x_{i-1}\Delta x_i)$ and is second order, that is if the grid spacing is decreased by 1/2, the T.E. error decreases by factor of 2^2. Thirdly, the previous point can be made clearer by focussing on the important case where the grid spacing is constant: $\Delta x_{i-1} = \Delta x_i = \Delta x$, the expression simplifies to:

$$\frac{u_{i+1} - u_{i-1}}{2\Delta x} - \left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{\Delta x^2}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \ldots \tag{11.22}$$

Hence, for an equally spaced grid the centered difference approximation converges quadratically as $\Delta x \to 0$:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2) \tag{11.23}$$

Note that like the forward and backward Euler difference formula, the centered difference uses information at only two points but delivers twice the order of the other two methods. This property will hold in general whenever the grid spacing is constant and the computational **stencil**, i.e. the set of points used in approximating the derivative, is symmetric.

11.3.2 Higher order approximation

The Taylor expansion provides a very useful tool for the derivation of higher order approximation to derivatives of any order. There are several approaches to achieve this. We will first look at an expendient one before elaborating on the more systematic one. In most of the following we will assume the grid spacing to be constant as is usually the case in most applications.

Equation (11.22) provides us with the simplest way to derive a fourth order approximation. An important property of this centered formula is that its truncation error contains only odd derivative terms:

$$\frac{u_{i+1} - u_{i-1}}{2\Delta x} = \frac{\partial u}{\partial x} + \frac{\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3} + \frac{\Delta x^4}{5!}\frac{\partial^5 u}{\partial x^5} + \frac{\Delta x^6}{7!}\frac{\partial^7 u}{\partial x^7} + \ldots + \frac{\Delta x^{2m}}{(2m+1)!}\frac{\partial^{(2m+1)} u}{\partial x^{(2m+1)}} + \ldots \tag{11.24}$$

The above formula can be applied with Δx replace by $2\Delta x$, and $3\Delta x$ respectively to get:

$$\frac{u_{i+2} - u_{i-2}}{4\Delta x} = \frac{\partial u}{\partial x} + \frac{(2\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3} + \frac{(2\Delta x)^4}{5!}\frac{\partial^5 u}{\partial x^5} + \frac{(2\Delta x)^6}{7!}\frac{\partial^7 u}{\partial x^7} + O(\Delta x^8) \tag{11.25}$$

$$\frac{u_{i+3} - u_{i-3}}{6\Delta x} = \frac{\partial u}{\partial x} + \frac{(3\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3} + \frac{(3\Delta x)^4}{5!}\frac{\partial^5 u}{\partial x^5} + \frac{(3\Delta x)^6}{7!}\frac{\partial^7 u}{\partial x^7} + O(\Delta x^8) \tag{11.26}$$

It is now clear how to combine the different estimates to obtain a fourth order approximation to the first derivative. Multiplying equation (11.24) by 2^2 and

substracting it from equation (11.25), we cancel the second order error term to get:

$$\frac{8(u_{i+1}-u_{i-1})-(u_{i+2}-u_{i-2})}{12\Delta x} = \frac{\partial u}{\partial x} - \frac{4\Delta x^4}{5!}\frac{\partial^5 u}{\partial x^5} - \frac{20\Delta x^6}{7!}\frac{\partial^7 u}{\partial x^7} + O(\Delta x^8) \quad (11.27)$$

Repeating the process for equation but using the factor 3^2 and substracting it from equation (11.26), we get

$$\frac{27(u_{i+1}-u_{i-1})-(u_{i+3}-u_{i-3})}{48\Delta x} = \frac{\partial u}{\partial x} - \frac{9\Delta x^4}{5!}\frac{\partial^5 u}{\partial x^5} - \frac{90\Delta x^6}{7!}\frac{\partial^7 u}{\partial x^7} + O(\Delta x^8) \quad (11.28)$$

Although both equations (11.27) and (11.28) are valid, the latter is not used in practice since it does not make sense to disregard neighboring points while using more distant ones. However, the expression is useful to derive a sixth order approximation to the first derivative: multiply equation (11.28) by 9 and equation (11.28) by 4 and substract to get:

$$\frac{45(u_{i+1}-u_{i-1})-9(u_{i+2}-u_{i-2})+(u_{i+3}-u_{i-3})}{60\Delta x} = \frac{\partial u}{\partial x} + \frac{36\Delta x^6}{7!}\frac{\partial^7 u}{\partial x^7} + O(\Delta x^8) \quad (11.29)$$

The process can be repeated to derive higher order approximations.

11.3.3 Remarks

The validity of the Taylor series analysis of the truncation error depends on the existence of higher order derivatives. If these derivatives do not exist, then the higher order approximations cannot be expected to hold. To demonstrate the issue more clearly we will look at specific examples.

Example 1 The function $u(x) = \sin \pi x$ is infinitely smooth and differentiable, and its first derivative is given by $u_x = \pi \cos \pi x$. Given the smoothness of the function we expect the Taylor series analysis of the truncation error to hold. We set about verifying this claim in a practical calculation. We lay down a computational grid on the interval $-1 \le x \le 1$ of constant grid spacing $\Delta x = 2/M$. The approximation points are then $x_i = i\Delta x - 1$, $i = 0, 1, \ldots, M$. Let ϵ be the error between the finite difference approximation to the first derivative, $\tilde{u}_x$, and its analytical derivative u_x:

$$\epsilon_i = \tilde{u}_x(x_i) - u_x(x_i) \quad (11.30)$$

The numerical approximation $\tilde{u}_x$ will be computed using the forward difference, equation (11.17), the backward difference, equation (11.20), and the centered difference approximations of order 2, 4 and 6, equations (11.22), (11.27, and (11.29). We will use two measures to characterize the error ϵ_i, and to measure its rate of decrease as the number of grid points is increased. One is a bulk measure and

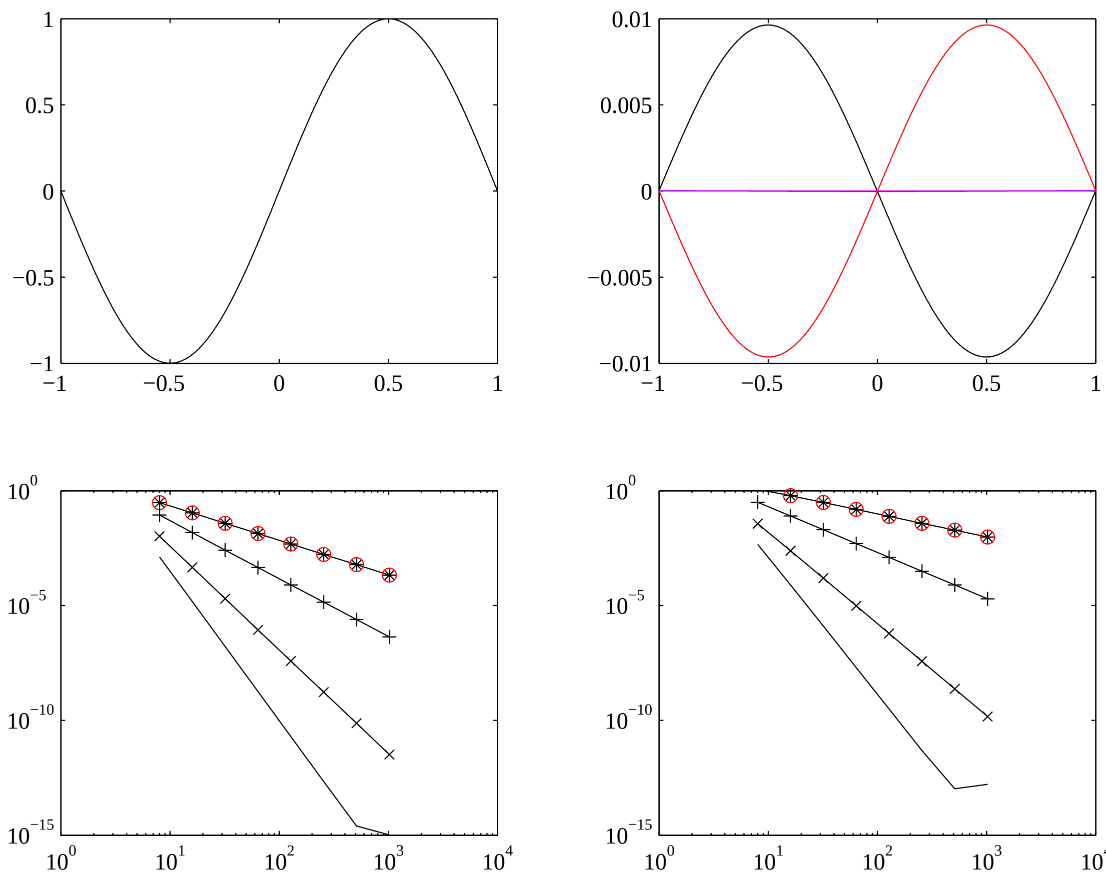

Figure 11.2: Finite difference approximation to the derivative of the function $\sin \pi x$. The top left panel shows the function as a function of x. The top right panel shows the spatial distribution of the error using the Forward difference (black line), the backward difference (red line), and the centered differences of various order (magenta lines) for the case $M = 1024$; the centered difference curves lie atop each other because their errors are much smaller then those of the first order schemes. The lower panels are convergence curves showing the rate of decrease of the rms and maximum errors as the number of grid cells increases.

consists of the root mean square error, and the other one consists of the maximum error magnitude. We will use the following notations for the rms and max errors:

$$\|\epsilon\|_2 = \Delta x \left(\sum_{i=0}^{M} \epsilon_i^2 \right)^{\frac{1}{2}} \tag{11.31}$$

$$\|\epsilon\|_\infty = \max_{0 \le i \le M} (|\epsilon_i|) \tag{11.32}$$

The right panel of figure 11.2 shows the variations of ϵ as a function of x for the case $M = 1024$ for several finite difference approximations to u_x. For the first order schemes the errors peak at $\pm 1/2$ and reaches 0.01. The error is much smaller for the higher order centered difference scheme. The lower panels of figure 11.2 show the decrease of the rms error ($\|\epsilon\|_2$ on the left), and maximum error ($\|\epsilon\|_\infty$ on the right) as a function of the number of cells M. It is seen that the convergence **rate** increases with an increase in the order of the approximation as predicted by the Taylor series analysis. The slopes on this log-log plot are -1 for forward and backward difference, and -2, -4 and -6 for the centered difference schemes of order 2, 4 and 6, respectively. Notice that the maximum error decreases at the same rate as the rms error even though it reports a higher error. Finally, if one were to gauge the efficiency of using information most accurately, it is evident that for a given M, the high order methods achieve the lowest error.

Example 2 We now investigate the numerical approximation to a function with finite differentiability, more precisely, one that has a discontinuous third derivative. This function is defined as follows:

	$u(x)$	$u_x(x)$	$u_{xx}(x)$	u_{xxx}
$x < 0$	$\sin \pi x$	$\pi \cos \pi x$	$-\pi^2 \sin \pi x$	$-\pi^3 \cos \pi x$
$0 < x$	$\pi x e^{-x^2}$	$\pi(1 - 2x^2)e^{-x^2}$	$2\pi x(2x^2 - 3)e^{-x^2}$	$-2\pi(3 - 12x^2 + 4x^4)e^{-x^2}$
$x = 0$	0	π	0	$-\pi^3, -6\pi$

Notice that the function and its first two derivatives are continuous at $x = 0$, but the third derivative is discontinuous. An examination of the graph of the function in figure 11.3 shows a curve, at least visually (the so called eye-ball norm). The error distribution is shown in the top right panel of figure 11.3 for the case $M = 1024$ and the fourth order centered difference scheme. Notice that the error is very small except for the spike near the discontinuity. The error curves (in the lower panels) show that the second order centered difference converges faster then the forward and backward Euler scheme, but that the convergence rates of the fourth and sixth order centered schemes are no better then that of the second order one. This is a direct consequence of the discontinuity in the third derivative whereby the Taylor expansion is valid only up to the third term. The effects of the discontinuity are more clearly seen in the maximum error plot (lower right panel) then in the mean error one (lower left panel). The main message of this example is that for

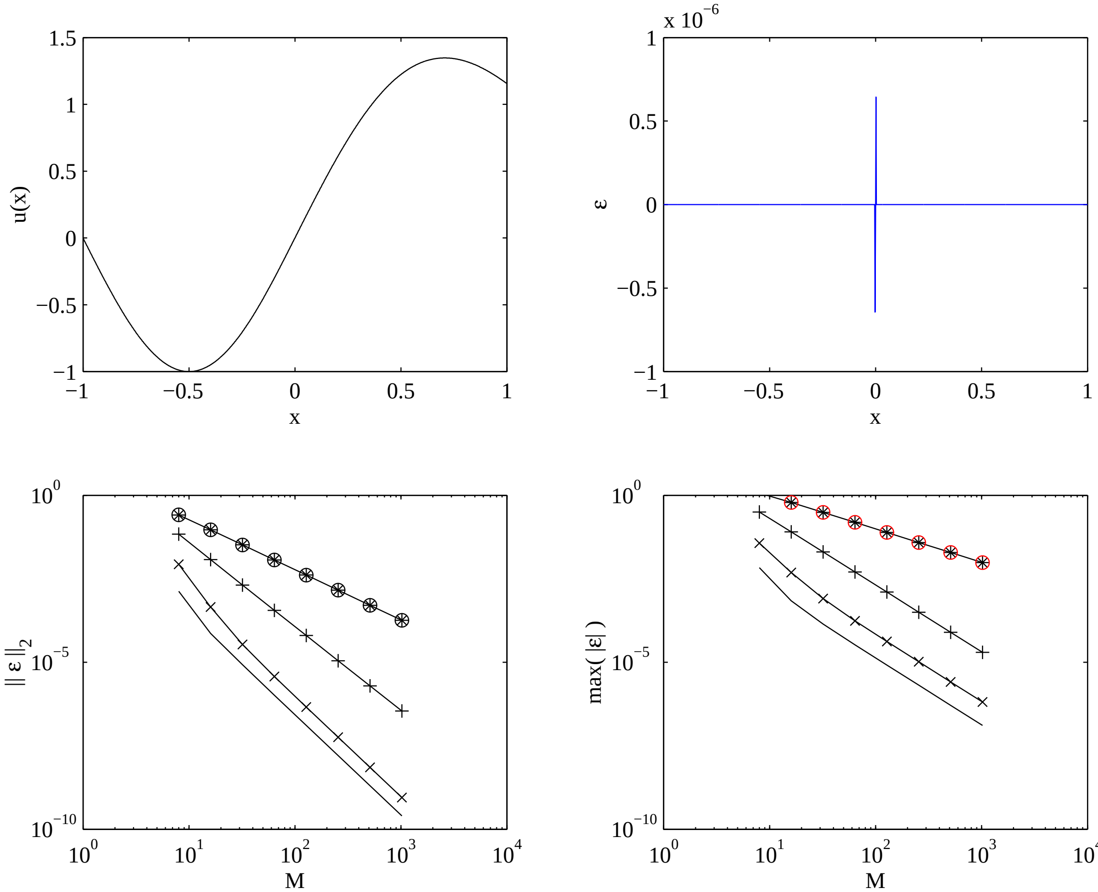

Figure 11.3: Finite difference approximation to the derivative of a function with discontinuous third derivative. The top left panel shows the function $u(x)$ which, to the eyeball norm, appears to be quite smooth. The top right panel shows the spatial distribution of the error ($M = 1024$) using the fourth order centered difference: notice the spike at the discontinuity in the derivative. The lower panels are convergence curves showing the rate of decrease of the rms and maximum errors as the number of grid cells increases.

functions with a finite number of derivatives, the Taylor series prediction for the high order schemes does not hold. Notice that the error for the fourth and sixth order schemes are lower then the other 3, but their **rate** of convergence is the same as the second order scheme. This is largely coincidental and would change according to the function.

11.3.4 Systematic Derivation of higher order derivative

The Taylor series expansion provides a systematic way of deriving approximation to higher order derivatives of any order (provided of course that the function is smooth enough). Here we assume that the grid spacing is uniform for simplicity. Suppose that the stencil chosen includes the points: x_j such that $i-l \le j \le i+r$. There are thus l points to the left and r points to the right of the point i where the derivative is desired for a total of $r+l+1$ points. The Taylor expansion is:

$$u_{i+m} = u_i + \frac{(m\Delta x)}{1!}u_x + \frac{(m\Delta x)^2}{2!}u_{xx} + \frac{(m\Delta x)^3}{3!}u_{xxx} + \frac{(m\Delta x)^4}{4!}u_{xxxx} + \frac{(m\Delta x)^5}{5!}u_{xxxxx} + \ldots \tag{11.33}$$

for $m = -l, \ldots, r$. Multiplying each of these expansions by a constant a_m and summing them up we obtain the following equation:

$$\begin{aligned}
\sum_{m=-l,m\neq 0}^{r} a_m u_{i+m} - \left(\sum_{m=-l,m\neq 0}^{r} a_m\right) u_i \;=\;& \left(\sum_{m=-l,m\neq 0}^{r} m a_m\right) \frac{\Delta x}{1!} \left.\frac{\partial u}{\partial x}\right|_i \\
&+ \left(\sum_{m=-l,m\neq 0}^{r} m^2 a_m\right) \frac{\Delta x^2}{2!} \left.\frac{\partial^2 u}{\partial x^2}\right|_i \\
&+ \left(\sum_{m=-l,m\neq 0}^{r} m^3 a_m\right) \frac{\Delta x^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_i \\
&+ \left(\sum_{m=-l,m\neq 0}^{r} m^4 a_m\right) \frac{\Delta x^4}{4!} \left.\frac{\partial^4 u}{\partial x^4}\right|_i \\
&+ \left(\sum_{m=-l,m\neq 0}^{r} m^5 a_m\right) \frac{\Delta x^5}{5!} \left.\frac{\partial^5 u}{\partial x^5}\right|_i \\
&+ \ldots
\end{aligned} \tag{11.34}$$

It is clear that the coefficient of the k-th derivative is given by $b_k = \sum_{m=-l,m\neq 0}^{r} m^k a_m$. Equation (11.34) allows us to determine the $r+l$ coefficients a_m according to the derivative desired and the order desired. Hence if the first order derivative is needed at fourth order accuracy, we would set b_1 to 1 and $b_{2,3,4} = 0$. This would provide us with four equations, and hence we need at least four points in order to determine its solution uniquely. More generally, if we need the k-th derivative then the

highest derivative to be neglected must be of order $k+p-1$, and hence $k+p-1$ points are needed. The equations will then have the form:

$$b_q = \sum_{m=-l,m\neq 0}^{r} m^q a_m = \delta_{qk}, q = 1,2,\ldots,k+p-1 \tag{11.35}$$

where δ_{qk} is the Kronecker delta $\delta_{qk} = 1$ is $q = k$ and 0 otherwise. For the solution to exit and be unique we must have: $l + r = k + p$. Once the solution is obtained we can determine the leading order truncation term by calculating the coefficient multiplying the next higher derivative in the truncation error series:

$$b_{k+1} \sum_{m=-l,m\neq 0}^{r} m^{k+p} a_m. \tag{11.36}$$

Example 3 As an example of the application of the previous procedure, let us fix the stencil to $r = 1$ and $l = -3$. Notice that this is an off-centered scheme. The system of equation then reads as follows in matrix form:

$$\begin{pmatrix} -3 & -2 & -1 & 1 \\ (-3)^2 & (-2)^2 & (-1)^2 & (1)^2 \\ (-3)^3 & (-2)^3 & (-1)^3 & (1)^3 \\ (-3)^4 & (-2)^4 & (-1)^4 & (1)^4 \end{pmatrix} \begin{pmatrix} a_{-3} \\ a_{-2} \\ a_{-1} \\ a_1 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} \tag{11.37}$$

If the first derivative is desired to fourth order accuracy, we would set $b_1 = 1$ and $b_{2,3,4} = 0$, while if the second derivative is required to third order accuracy we would set $b_{1,3,4} = 0$ and $b_2 = 1$. The coefficients for the first example would be:

$$\begin{pmatrix} a_{-3} \\ a_{-2} \\ a_{-1} \\ a_1 \end{pmatrix} = \frac{1}{12} \begin{pmatrix} -1 \\ 12 \\ -18 \\ 3 \end{pmatrix} \tag{11.38}$$

11.3.5 Discrete Operator

Operators are often used to describe the discrete transformations needed in approximating derivatives. This reduces the lengths of formulae and can be used to derive new approximations. We will limit ourselves to the case of the centered difference operator:

$$\delta_{nx} u_i = \frac{u_{i+\frac{n}{2}} - u_{i-\frac{n}{2}}}{n\Delta x} \tag{11.39}$$

$$\delta_{x} u_i = \frac{u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}}{\Delta x} = u_x + O(\Delta x^2) \tag{11.40}$$

$$\delta_{2x} u_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} = u_x + O(\Delta x^2) \tag{11.41}$$

The second order derivative can be computed by noticing that

$$\begin{aligned}
\delta_x^2 u_i = \delta_x(\delta_x u_i) &= \delta_x(u_x + O(\Delta x^2)) && (11.42)\\
\delta_x\left(\frac{u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}}{\Delta x}\right) &= u_{xx} + O(\Delta x^2) && (11.43)\\
\frac{1}{\Delta x}\left(\delta_x(u_{i+\frac{1}{2}}) - \delta_x(u_{i-\frac{1}{2}})\right) &= u_{xx} + O(\Delta x^2) && (11.44)\\
\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}) &= u_{xx} + O(\Delta x^2) && (11.45)
\end{aligned}$$

The truncation error can be verified by going through the formal Taylor series analysis.

Another application of operator notation is the derivation of higher order formula. For example, we know from the Taylor series that

$$\delta_{2x} u_i = u_x + \frac{\Delta x^2}{3!} u_{xxx} + O(\Delta x^4) \qquad (11.46)$$

If I can estimate the third order derivative to second order then I can substitute this estimate in the above formula to get a fourth order estimate. Applying the δ_x^2 operator to both sides of the above equation we get:

$$\delta_x^2(\delta_{2x} u_i) = \delta_x^2(u_x + \frac{\Delta x^2}{3!} u_{xxx} + O(\Delta x^4)) = u_{xxx} + O(\Delta x^2) \qquad (11.47)$$

Thus we have

$$\delta_{2x} u_i = u_x + \frac{\Delta x^2}{3!}\delta_x^2[\delta_{2x} u_i + O(\Delta x^2)] \qquad (11.48)$$

Rearranging the equation we have:

$$u_x|_{x_i} = \left(1 - \frac{\Delta x^3}{3!}\delta_x^2\right)\delta_{2x} u_i + O(\Delta x^4) \qquad (11.49)$$

11.4 Polynomial Fitting

Taylor series expansion are not the only means to develop finite difference approximation. An another approach is to rely on polynomial fitting such as splines (which we will not discuss here), and Lagrange interpolation. We will concentrate on the later in the following section.

Lagrange interpolation consists of fitting a polynomial of a specified defree to a given set of (x_i, u_i) pairs. The slope at the point x_i is approximated by taking the derivative of the polynomial at the point. The approach is best illustrate by looking at specific examples.

11.4.1 Linear Fit

The linear polynomial:

$$L_1(x) = \frac{x - x_i}{\Delta x} u_{i+1} - \frac{x - x_{i+1}}{\Delta x} u_i, \quad x_i \leq x \leq x_{i+1} \tag{11.50}$$

The derivative of this function yields the forward difference formula:

$$u_x|_{x_i} = \left.\frac{\partial L_1(x)}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_i}{\Delta x} \tag{11.51}$$

A Taylor series analysis will show this approximation to be linear. Likewise if a linear interpolation is used to interpolate the function in $x_{i-1} \leq x \leq x_i$ we get the backward difference formula.

11.4.2 Quadratic Fit

It is easily verified that the following quadratic interpolation will fit the function values at the points x_i and $x_{i\pm1}$:

$$L_2(x) = \frac{(x - x_i)(x - x_{i+1})}{2\Delta x^2} u_{i-1} - \frac{(x - x_{i-1})(x - x_{i+1})}{\Delta x^2} u_i + \frac{(x - x_{i-1})(x - x_i)}{2\Delta x^2} u_{i+1} \tag{11.52}$$

Differentiating the functions and evaluating it at x_i we can get expressions for the first and second derivatives:

$$\left.\frac{\partial L_2}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} \tag{11.53}$$

$$\left.\frac{\partial^2 L_2}{\partial x^2}\right|_{x_i} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \tag{11.54}$$

Notice that these expression are identical to the formulae obtained earlier. A Taylor series analysis would confirm that both expression are second order accurate.

11.4.3 Higher order formula

Higher order fomula can be develop by Lagrange polynomials of increasing degree. A word of caution is that high order Lagrange interpolation is practical when the evaluation point is in the **middle of the stencil**. High order Lagrange interpolation is notoriously noisy near the end of the stencil when equal grid spacing is used, and leads to the well known problem of Runge oscillations [1]. Spectral methods that do not use periodic Fourier functions (the usual “sin” and “cos” functions) rely on **unevenly** spaced points.

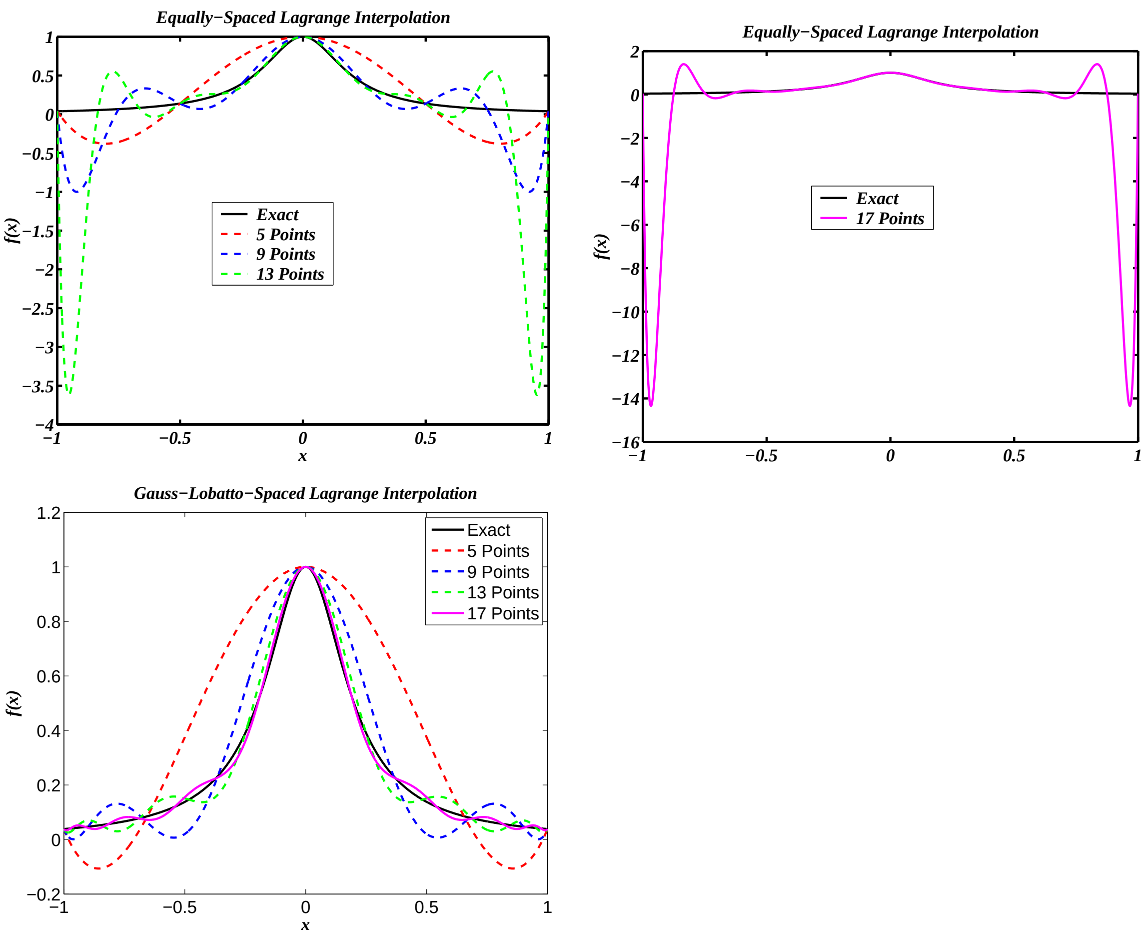

Figure 11.4: Illustration of the Runge phenomenon for equally-spaced Lagrangian interpolation (upper figures). The right upper figure illustrate the worsening amplitude of the oscillations as the degree is increased. The Runge oscillations are suppressed if an unequally spaced set of interpolation point is used (lower panel); here one based on Gauss-Lobatto roots of Chebyshev polynomials. The solution black line refers to the exact solution and the dashed lines to the Lagrangian interpolants. The location of the interpolation points can be guessed by the crossing of the dashed lines and the solid black line.

To illustrate the Runge phenomenon we'll take the simple example of interpolating the function

$$f(x) = \frac{1}{1 + 25x^2} \tag{11.55}$$

in the interval $|x| \leq 1$. The Lagrange interpolation using an equally spaced grid is shown in the upper panel of figure 11.4, the solid line refers to the exact function f while the dashed-colored lines to the Lagrange interpolants of different orders. In the center of the interval (near $x = 0$, the difference between the dashed lines and the solid black line decreases quickly as the polynomial order is increased. However, near the edges of the interval, the Lagrangian interpolants oscillates between the interpolation points. At a fixed point near the boundary, the oscillations' amplitude becomes bigger as the polynomial degree is increased: the amplitude of the 16 order polynomial reaches of value of 17 and has to be plotted separately for clarity of presentation. This is not the case when a non-uniform grid is used for the interpolation as shown in the lower left panel of figure 11.4. The interpolants approach the true function in the center and at the edges of the interval. The points used in this case are the Gauss-Lobatto roots of the Chebyshev polynomial of degree $N - 1$, where N is the number of points.