Chapter 3. Numerical Differentiation

3.1. Introduction

The ability to numerically evaluate derivatives at particular points is important in several applications. Sometimes we have experimental data for concentration as a function of time. However, our models are based on reaction rates, that is the change in concentration as a function of time. Therefore, in order to make a direct comparison between the experimental data and the model, we must either integrate the model or differentiate the data. For the time being, we will postpone judgment on the relative merits of the two options. We shall be content to be able to perform either option as need dictates.

There are also situations in the solution of nonlinear algebraic equations where having derivatives are desirable but the analytical forms of the functions are unavailable. In this case, again, we must rely on numerical differentiation.

3.2. Taylor Series Expansions

Many of the most common formulae for numerical derivatives are derived from a Taylor Series Expansion. As a reminder, a Taylor Series expansion of a function $f(x)$, about a point, x_0, is given by

$$f(x) = f(x_0) + \left.\frac{df}{dx}\right|_{x_0} (x - x_0) + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x_0} (x - x_0)^2 + \ldots + \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x_0} (x - x_0)^n + \ldots \qquad (3.1.a)$$

or equivalently as

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x_0} (x - x_0)^n \qquad (3.1.b)$$

Frequently, we assume that the x-axis is discretized into points. The step size, $(x_{i+1} - x_i)$, is replaced with the variable *h*, leaving in which case the Taylor series expansion can be written as

$$f(x_{i+1}) = f(x_i) + \left.\frac{df}{dx}\right|_{x_i} h + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x_i} h^2 + \ldots + \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x_i} h^n + \ldots \qquad (3.1.c)$$

In practice the Taylor Series is truncated after a particular term so that one has an error of the order of first missing term,

$$f(x_{i+1}) = \sum_{n=0}^{m} \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x_i} h^n + O\left(h^{m+1}\right) \qquad (3.1.d)$$

3.3. Finite Difference Formulae

Taylor Series are used to derive formula for numerical derivatives. There are an infinite number of formulae. We will derive a few common formula. Remember as we do this that we can derive equations for different levels of derivative, the first derivative, the second derivative etc. We can also derive equations with different orders of error, depending upon where we truncate the series. Longer (higher order) series provide more accurate estimates of the derivative. Third, we can choose in which direction to expand the Taylor series, forward (in the positive x direction), backward (in the negative x direction) or centered (in both positive and negative x directions). These three choices lead to a myriad of formula; for example one can have a second order numerical formula for the first derivative in the forward direction.

We begin with first derivatives. If we truncate the Taylor Series at the first order term we have

$$f(x_{i+1}) = f(x_i) + \left.\frac{df}{dx}\right|_{x_i} h + O\left(h^2\right) \qquad (3.2)$$

Solving for the derivative yields

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \qquad (3.3)$$

where it can be shown that the truncated term is now of order 1. Thus equation (3.3) provides the first-order forward finite difference formula for the first derivative.

If we take the Taylor series in the negative x-direction, we have an analogous expression

$$f(x_{i-1}) = f(x_i) - \left.\frac{df}{dx}\right|_{x_i} h + O(h^2) \tag{3.4}$$

Solving for the derivative yields

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_i) - f(x_{i-1})}{h} + O(h) \tag{3.5}$$

Thus we have the first-order backward finite difference formula for the first derivative. If we subtract equation (3.4) from equation (3.2) we obtain

$$f(x_{i+1}) - f(x_{i-1}) = 2\left.\frac{df}{dx}\right|_{x_i} h + O(h^3) \tag{3.6}$$

The error in this expression is of order h^3 because the $O(h^2)$ terms cancelled. Rearranging for the derivative yields

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \tag{3.7}$$

Thus we have a second order centered finite difference formula for the first derivative. In all of these expressions we estimate the value of the first derivative based on function evaluations alone.

This general procedure for using the Taylor Series to generate estimates for derivatives can be applied to generate higher order approximations for higher order derivatives. We shall simply state that the lowest order formulae for the second derivatives are for the forward finite difference,

$$\left.\frac{d^2 f}{dx^2}\right|_{x_i} = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h\ ) \tag{3.8.a}$$

for the reverse finite difference,

$$\left.\frac{d^2 f}{dx^2}\right|_{x_i} = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} + O(h\ ) \tag{3.8.b}$$

and for the centered finite difference,

$$\left.\frac{d^2 f}{dx^2}\right|_{x_i} = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2) \tag{3.8.c}$$

The next higher order expressions for the first derivatives are for the forward finite difference,

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2) \tag{3.9.a}$$

for the reverse finite difference,

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} + O(h^2) \tag{3.9.b}$$

and for the centered finite difference,

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + O(h^4) \tag{3.9.c}$$

The next higher order expressions for the second derivatives are for the forward finite difference,

$$\left.\frac{d^2 f}{dx^2}\right|_{x_i} = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} + O(h^2) \tag{3.10.a}$$

for the reverse finite difference,

$$\left.\frac{d^2 f}{dx^2}\right|_{x_i} = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2} + O(h^2) \tag{3.10.b}$$

and for the centered finite difference,

$$\left.\frac{d^2 f}{dx^2}\right|_{x_i} = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} + O(h^4) \tag{3.10.c}$$

Formulae for higher order derivatives are available elsewhere.[Chapra & Canale, 1988.]

3.4. Approximations for Partial Derivatives

Finite difference formulae exist for partial derivatives of functions of more than one variable. We simply report a few of the most useful formulae here. The expression for the first derivatives do not change in form. For example the centered finite difference formula for the ordinary differential given in equation (3.7)

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \tag{3.7}$$

becomes for partial derivative with respect to variable x_j

$$\left.\left(\frac{df}{dx_j}\right)_{x_{k\neq j}}\right|_{x_j^{(i)}} = \frac{f\left(x_1^{(i)} \ldots x_j^{(i+1)} \ldots x_n^{(i)}\right) - f\left(x_1^{(i)} \ldots x_j^{(i-1)} \ldots x_n^{(i)}\right)}{2h_j} + O\left(h_j^2\right) \tag{3.11}$$

Let it be clear that the j subscript on the variable x indicates a different independent variable. The superscript (i) on the x is not an exponent. The parentheses are included to make clear it is a notation that does not signify a mathematical operation. Instead, the superscript (i) indicates a different value of x, which we shall soon see can be associated with the i-1, i and i+1 nodes. The subscript that now appears outside the parentheses, $x_{k\neq j}$, indicates that all variables except x_j are held constant in the differentiation. The final subscript $x_j^{(i)}$ of the partial derivative indicates the value of x_j where the derivative is evaluated.

The second partial derivative with respect to variable x_j is analogous to the centered finite difference formula for the ordinary second differential given in equation (3.8.c)

$$\left.\frac{d^2 f}{dx^2}\right|_{x_i} = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2) \tag{3.8.c}$$

becomes

$$\left.\left(\frac{\partial^2 f}{\partial x_j^2}\right)_{x_{k\neq j}}\right|_{x_j^{(i)}} = \frac{f\left(x_1^{(i)} \ldots x_j^{(i+1)} \ldots x_n^{(i)}\right) - 2f\left(x_1^{(i)} \ldots x_j^{(i)} \ldots x_n^{(i)}\right) + f\left(x_1^{(i)} \ldots x_j^{(i-1)} \ldots x_n^{(i)}\right)}{h_j^2} + O\left(h_j^2\right) \tag{3.12}$$

Finally, the mixed second partial derivative with respect to variables x_j and x_m is

$$\left.\left(\frac{\partial}{\partial x_m}\left(\frac{\partial f}{\partial x_j}\right)_{x_{k\neq j}}\right)_{x_{k\neq m}}\right|_{x_j^{(i)},x_m^{(i)}} = \frac{\begin{bmatrix} f\left(x_1^{(i)}\ldots x_j^{(i+1)},x_m^{(i+1)}\ldots x_n^{(i)}\right) - f\left(x_1^{(i)}\ldots x_j^{(i+1)},x_m^{(i-1)}\ldots x_n^{(i)}\right) \\ - f\left(x_1^{(i)}\ldots x_j^{(i-1)},x_m^{(i+1)}\ldots x_n^{(i)}\right) + f\left(x_1^{(i)}\ldots x_j^{(i-1)},x_m^{(i-1)}\ldots x_n^{(i)}\right)\end{bmatrix}}{4h_j h_m} + O\left(h_j h_m\right) \quad (3.13)$$

which is symmetric with respect to the order of differentiation,

$$\left.\left(\frac{\partial}{\partial x_m}\left(\frac{\partial f}{\partial x_j}\right)_{x_{k\neq j}}\right)_{x_{k\neq m}}\right|_{x_j^{(i)},x_m^{(i)}} = \left.\left(\frac{\partial}{\partial x_j}\left(\frac{\partial f}{\partial x_m}\right)_{x_{k\neq m}}\right)_{x_{k\neq j}}\right|_{x_m^{(i)},x_j^{(i)}} \quad (3.14)$$

3.5. Noise

Life is noisy. There is always uncertainty associated with the measurements of data. Nowhere is the impact of noise in the data more evident than in numerical differentiation. To illustrate this point, we shall apply some of the formulae presented in the previous section and observe their accuracy as a function of the amount of noise in the data.

We shall investigate a toy problem, with a simple monotonically increasing function, $f(x) = x^2 + x^3$, along a small range, from 0 to 1. The function is shown without any noise in Figure 3.1. It is plotted with a data discretization of 0.01 in the x-direction. Also shown is the function with varying degrees of noise ranging from 0.01% to 20% noise. The noise is randomly generated at each data point.

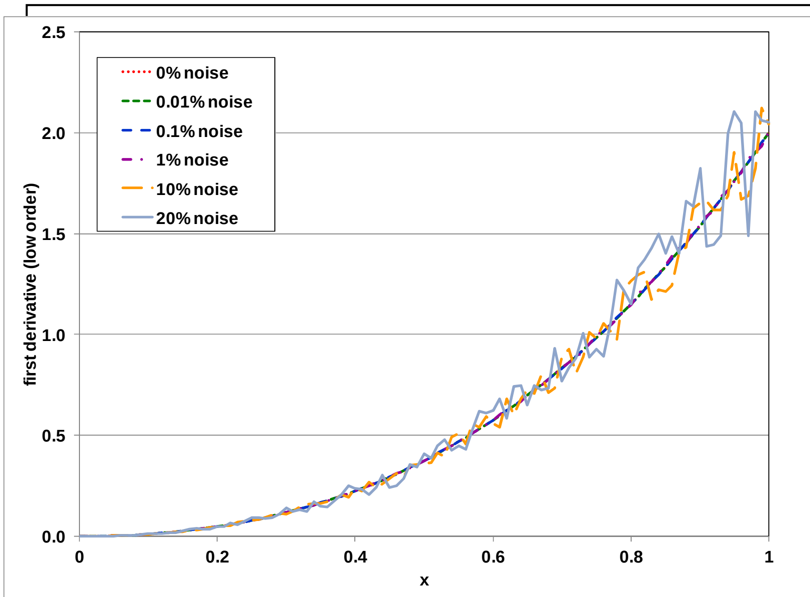

Figure 3.1. A plot of $f(x) = x^2 + x^3$ with varying degrees of noise in the data.

We shall investigate the effect of noise on centered-finite difference formulae, although the conceptual results is the same for the forward and backward finite difference formulae. We presented four centered finite difference formula in the previous section: (i) a second-order approximation to the first derivative, equation (3.7), (ii) a fourth-order approximation to the first derivative, equation (3.9.c), (iii) a second order approximation to the second derivative, equation (3.8.c) and (iv) a fourth order approximation to the second derivative, equation (3.10.c). In Figure 3.2, we present two plots for each of the four finite difference formulae. The first plot is of the derivative itself. The second plot is presented on a semi-log plot and presents the absolute value of the relative error of the derivative referenced to the analytical value of the derivative.

We begin the discussion by noting that the function in Figure 3.1 retains the correct shape, despite the presence of noise. In practice we may judge this data to be fairly good, especially for the lower percentages of noise. However, the derivatives plotted on the left side of Figure 3.2 tell a very different story. What instantly stands out is that the derivatives can easily have the wrong sign, giving the impression that the function is not monotonically increasing, nor always of positive concavity. For all four approximations, we observe from the error plotted on a log axis on the right side that that the error of the approximate derivative increases as the noise increases. In this error plot, a value of 1 corresponds to 100% error. We note that the higher order methods do not demonstrate an appreciable improvement over the lower order methods for noisy data.

Also of note, we observe for the second-order approximation of the first derivative, that there is an error in the derivative even based on the original function with no noise in the range from 10^{-3} to 10^{-5}. This is a measure of the accuracy of the formulae. The polynomial is third order and the formulae is second order so the approximation is not exact. However, when we apply the fourth-order approximation to the first derivative, we find that the error drops to 10^{-16}. The finite difference formuala should be exact. Our calculations only include 16 digits. This error is due to “truncation error” due to the finite precision of our software.

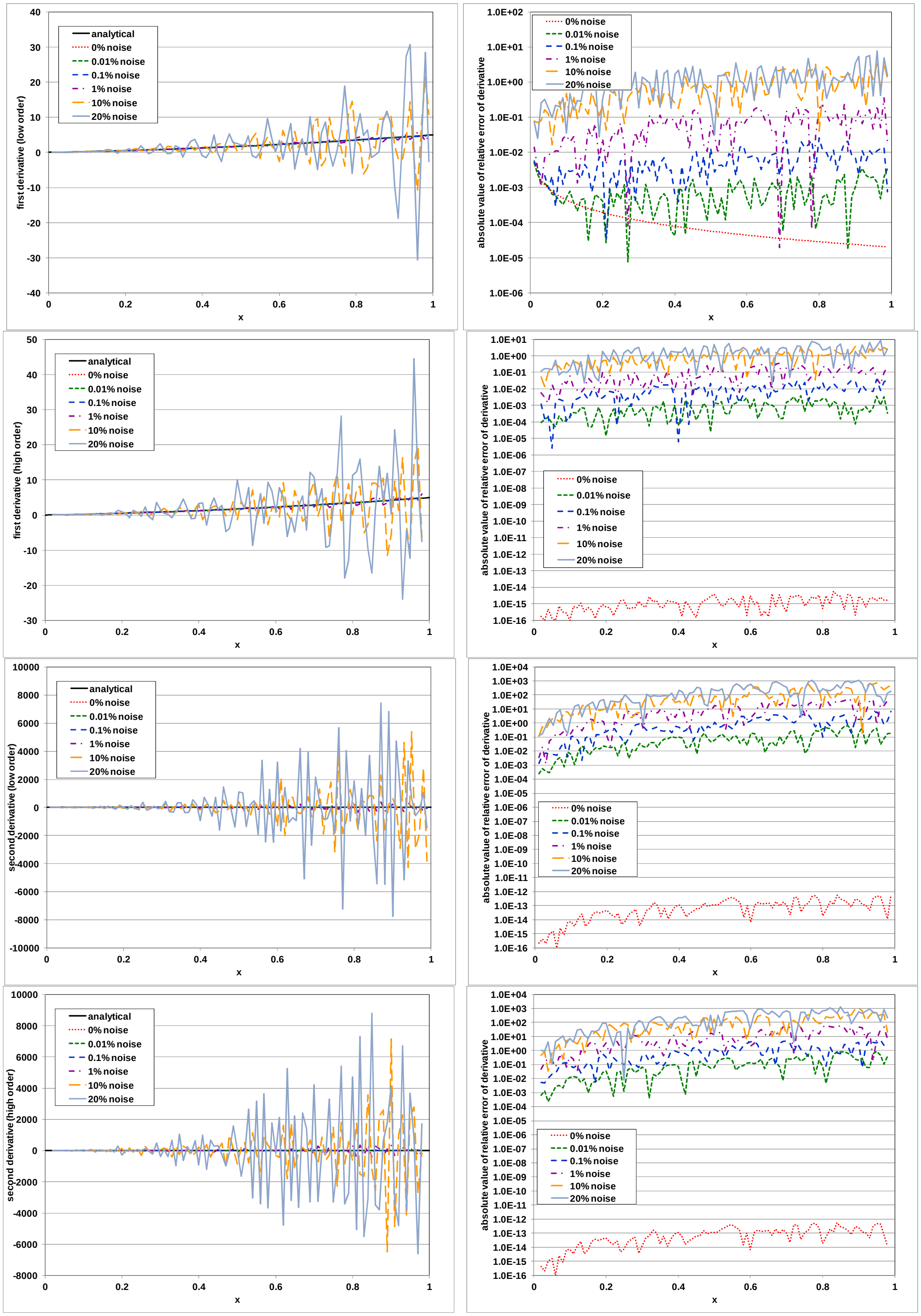

Figure 3.2. Affect of noise on numerical differentiation of centered finite difference formulae.

3.6. Problems

Problems are located on course website.