Chapter 3

§1 Numerical Differentiation

Differentiation and integration are infinitary concepts of calculus; that is they are defined by means of a limit process – the limit of the difference quotient, and the limit of Riemann sums. Since limit processes cannot be carried out on the computer, we must replace them by finite processes.

Goal : For a given differentiable function f, we want to approximate the derivative $f^{'}(x)$ in terms of the values of f at x_0 and near by points $x_0, \ldots, x_n$ (Not necessarily equally spaced or in natured order).

§1.1 A general differentiation formula for unequally spaced

Idea : Simply to differentiate not $f(\cdot)$, but its interpolation polynomial $p_n(f : x_0, \ldots, x_n; \cdot)$.

Given n+1 distinct points, we have

$$f(x) = p_n(f; x) + r_n(x),$$

where

$$\begin{aligned} p_n(f;x) &= f_0 + (x - x_0)[x_0, x_1]f + (x - x_0)(x - x_1)[x_0, x_1, x_2]f \\ &\quad + \cdots + (x - x_0) \cdots (x - x_{n-1})[x_0, x_1, \cdots, x_n]f \end{aligned}$$

$$r_n(x) = (x - x_0)(x - x_1) \cdots (x - x_n) \frac{f^{(n+1)}(\xi(x))}{(n+1)!},$$

note that we need to assume f has in fact n+2 continuous derivatives, then we get

$$\begin{aligned} p_n^{'}(f; x_0) &= [x_0, x_1]f + (x_0 - x_1)[x_0, x_1, x_2]f + \cdots \\ &\quad + (x_0 - x_1) \cdots (x_0 - x_{n-1})[x_0, x_1, \cdots, x_n]f \end{aligned}$$

$$r_n'(x_0) = (x_0 - x_1)\cdots(x_0 - x_n)\frac{f^{(n+1)}(\xi(x_0))}{(n+1)!} \equiv e_n$$

Therefore $f'(x_0) = p_n'(f; x_0) + e_n$

if H = $\max_i |x_0 - x_i|$, then

$$e_n = O(H^n) \text{ as } H \to 0$$

§1.2 Examples

Example:

$$n = 1, x_1 = x_0 + h$$

$$p_1'(f; x_0) = [x_0, x_1]f = \frac{f_1 - f_0}{h}$$

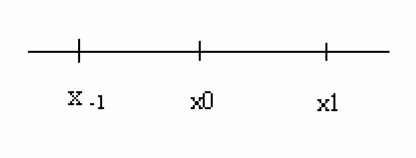
$$f'(x_0) = \frac{f_1 - f_0}{h} + e_0,$$

$$e_1 = -h\frac{f''(\xi)}{2} \quad \text{provided} \quad f \in C^3[x_0, x_1].$$
$$e_1 = O(h) \quad h \to 0.$$

Taylor's formula, actually, shows that $f \in C^2[x_0, x_1]$ suffices.

Example:

n=2,



$$p_2'(f;x_0) = [x_0, x_1]f + (x_0 - x_1)[x_0, x_1, x_2]f.$$

$$\begin{array}{llll}
x_{-1} & f_{-1} & & \\
x_0 & f_0 & \dfrac{f_0 - f_{-1}}{h} & \\
x_1 & f_1 & \dfrac{f_1 - f_0}{h} & \dfrac{f_1 - 2f_0 + f_{-1}}{2h^2}
\end{array}$$

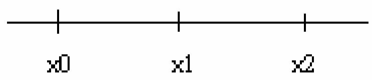
$$\therefore p_2'(f;x_0) = \frac{f_1 - f_0}{h} - h\frac{f_1 - 2f_0 + f_{-1}}{2h^2} = \frac{f_1 - f_{-1}}{2h}$$

$$f'(x_0) = \frac{f_1 - f_{-1}}{2h} + e_2, \qquad e_2 = -h^2\frac{f'''(\xi)}{6}$$

$$e_2 = O(h^2) \qquad \text{as} \quad h \longrightarrow 0$$

$-\,-$ centeral difference

Example:
n=2,



$$\begin{array}{llll} x_0 & f_0 & & \\ x_1 & f_1 & \dfrac{f_1-f_0}{h} & \\ x_2 & f_2 & \dfrac{f_2-f_1}{h} & \dfrac{f_2-2f_1+f_0}{2h^2} \end{array}$$

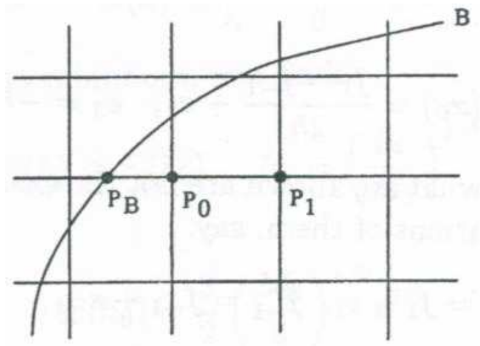
$$\therefore p_2^{'}(f;x_0) = \frac{f_1-f_0}{h} - h\frac{f_2-2f_1+f_0}{2h^2} = \frac{-f_2+4f_1-3f_0}{2h}$$

$$f^{'}(x_0) = \frac{-f_2+4f_1-3f_0}{2h} + e_2, \qquad e_2 = -h^2\frac{f^{'''}(\xi)}{3}$$

Remark : bigger error due to destroying symmetry.

Example:

For a function $u = u(x, y)$ of two variables, approximate $\frac{\partial u}{\partial x}(P_0)$ near the boundary. Consider the points $P_0(x_0, y_0), P_1(x_0+h, y_0), P_B(x_0-\beta h, y_0)$, $0 < \beta < 1$.



Let $\quad u_0 = u(P_0) \quad u_1 = u(P_1) \quad u_B = u(P_B)$

$$
\begin{array}{llcc}
x_B & u_B & & \\
x_0 & u_0 & \dfrac{u_0 - u_B}{\beta h} & \\
x_1 & u_1 & \dfrac{u_1 - u_0}{h} & \dfrac{\beta(u_1 - u_0) - (u_0 - u_B)}{\beta h(1+\beta)h}
\end{array}
$$

Thus

$$
\begin{aligned}
p_2'(u; P_0) &= \frac{u_1 - u_0}{h} - h\frac{\beta(u_1 - u_0) - (u_0 - u_B)}{\beta h(1+\beta)h} \\
&= \frac{\beta^2 u_1 + (1-\beta^2)u_0 - u_B}{\beta(1+\beta)h}
\end{aligned}
$$

$$
e_2 = -\frac{\beta}{6}h^2\frac{\partial^3 u}{\partial x^3}(\xi, y_0)
$$

§1.3 Numerical differentiation with perturbed data

Formulae for numerical differentiation become more accurate as the spacing h between evaluation points is made smaller, provided the function to be differentiated is sufficiently smooth. This, however, is true only in theory, since in practice the data are usually inaccurate, if no other reason than rounding, and the problem of cancellation becomes more acute as h gets smaller. There will be a point of diminishing returns, beyond which the errors increase rather than decrease, i.e. in theory, formulae for numerical differentiation become more accurate as h is made smaller. But cancellation effects occur as h gets smaller.

Let's take the center difference formula :

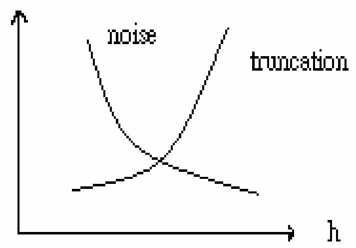
$$f'(x_0) = \frac{f_1 - f_{-1}}{2h} + e_2, \qquad e_2 = -h^2 \frac{f'''(\xi)}{6}$$

$$\text{let} \quad f_1^* = f_1 + \varepsilon_1, \quad f_{-1}^* = f_{-1} + \varepsilon_{-1}, \quad |\varepsilon_{\pm 1}| \leq \varepsilon$$

$$\therefore f'(x_0) = \frac{f_1^* - f_{-1}^*}{2h} - \frac{\varepsilon_1 - \varepsilon_{-1}}{2h} + e_2$$

$$E_2 = f'(x_0) - \frac{f_1^* - f_{-1}^*}{2h} = -\frac{\varepsilon_1 - \varepsilon_{-1}}{2h} + e_2$$

$$|E_2| \leq \underbrace{\frac{\varepsilon}{h}}_{\text{noise}} + \underbrace{\frac{M_3}{6} h^2}_{\text{truncation}}, \qquad M_3 = \max_{[x_{-1}, x_1]} |f'''|$$



Let $E(h) = \dfrac{\varepsilon}{h} + \dfrac{M_3}{6}h^2 \quad h_0 = \left(\dfrac{3\varepsilon}{M_3}\right)^{\frac{1}{3}}$

$E(h_0) = \dfrac{3}{2}\left(\dfrac{M_3}{3}\right)^{\frac{1}{3}}\varepsilon^{\frac{2}{3}}$ is the minimum

then $E \sim O(\varepsilon^{\frac{2}{3}})$

not $O(\varepsilon)$ as one would hope

Alternative: Cauchy's formula

Use not difference formulae, but summation formulae, that is, integration

$$f'(x_0) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{(z-x_0)^2}dz = \frac{1}{2\pi r}\int_0^{2\pi} e^{-i\theta} f(x_0 + re^{i\theta})d\theta$$

Remark: Need f to be able to analytically extend to complex plane.