Chapter 6 Numerical Differentiation

6.1 Approximating The Derivative

Approximating the derivative of $f(x)$

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

Choose a sequence $\{h_k\}$ so that $h_k \to 0$ and compute the limit of the sequence:

$$D_k = \frac{f(x+h_k) - f(x)}{h_k} \qquad \text{for } k = 1, 2, ..., n, ...$$

Example: Let $f(x) = x^2$ and $x = 1$. Compute the difference quotients D_k using step size $h_k = 10^{-k}$ for $k = 1, 2, ..., 10$. Carry out nine decimal places in all calculations

```
function ExDer
    x = -1 : 0.1 : 2;
    y = exp (x);
    plot (x, y);

    x0 = 1;
    fprintf('\th\t\tDk = (fk - e)/hk\n');
    table = [];
    for k = 1 : 10
        h = 10^-k;
        D(k) = (exp (x0 + h) - exp (x0)) / h;
        table = [table; h, D(k)];
    end

    disp (table);
end
```

The Central-difference Formula

Theorem (Centered Formula of Order $O(h^2)$). Assume that $f \in C^3[a,b]$ and that $x-h, x, x+h \in [a,b]$, then

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

Furthermore, there exists a number $c \in [a,b]$ such that

$$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h} + E_{trunc}(f,h)$$

where

$$E_{trunc}(f,h) = -\frac{h^2 f^{(3)}(c)}{6} = O(h^2)$$

The term $E_{trunc}(f,h)$ is called **truncation error**.

Proof: Taylor expansions about x for $f(x+h)$ and $f(x-h)$

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(c1)h^3}{3!}$$

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(c2)h^3}{3!}$$

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{((f^{(3)}(c1)+f^{(3)}(c2)))h^3}{3!}$$

since $f^{(3)}(x)$ is continuous, the intermediate value theorem can be used to find c so that

$$\frac{f^{(3)}(c1)+f^{(3)}(c2)}{2} = f^{(3)}(c)$$

rearrange to yield

$$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h} - \frac{h^2 f^{(3)}(c)}{6}$$

Theorem (Centered Formula of Order $O(h^4)$). Assume that $f \in C^5[a, b]$ and that $x - 2h, x - h, x, x + h, x + 2h \in [a, b]$, then

$$f'(x) \approx \frac{-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)}{12h}$$

Furthermore, there exists a number $c \in [a, b]$ such that

$$f'(x) = \frac{-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)}{12h} + E_{trunc}(f, h)$$

where

$$E_{trunc}(f, h) = \frac{h^4 f^{(5)}(c)}{30} = O(h^4)$$

Example: Let $f(x) = cos(x)$, with step size $h = 0.1, 0.01, 0.001, 0.0001$

6.2 Numerical Differentiation Formulas

Central-difference formulas of order $O(h^2)$

$$f'(x_0) = \frac{f_1 - f_{-1}}{2h}$$

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

$$f^{(3)}(x_0) = \frac{f_2 - f_1 + 2f_{-1} + f_{-2}}{2h^3}$$

$$f^{(4)}(x_0) = \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4}$$

Central-difference formulas of order $O(h^4)$

$$f'(x_0) = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}$$

$$f''(x_0) = \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} + f_{-2}}{12h^2}$$

$$f^{(3)}(x_0) = \frac{-f_3 + 8f_2 - 13f_1 + 13f_{-1} - 8f_{-2} + f_{-3}}{8h^3}$$

$$f^{(4)}(x_0) = \frac{-f_3 + 12f_2 - 39f_1 + 56f_0 - 39f_{-1} + 12f_{-2} - f_{-3}}{6h^4}$$