Section 6.2 Numerical Differentiation Part 2

Another basic problem in numerical differentiation is stated as:

Derive a formula that approximates the derivative of a function in terms of a linear combination of function values.

Although the formulas developed in this section can be used to estimate the value of a derivative at a particular value in the domain of a function, they are primarily used in the solution of differential equations in what called **finite difference methods**.

Difference Approximations to Derivatives

A **difference quotient** is a change in function values divided by the corresponding domain values. For example

$$\frac{\Delta y}{\Delta x} = \frac{y_1 - y_0}{x_1 - x_0}.$$

For y = f(x) with x = x_0 and x_1 we have

$$\frac{\Delta y}{\Delta x} = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

or for y = f(x) with x = x_0 and $x_1 = x_0 + h$ we have

$$\frac{\Delta y}{\Delta x} = \frac{f(x_0 + h) - f(x_0)}{x_0 + h - x_0} = \frac{f(x_0 + h) - f(x_0)}{h}.$$

Forward Difference Approximation

Given **y = f(x)** and $y_h = \frac{f(x_0 + h) - f(x_0)}{h}$ for h > 0 and some fixed value x_0. Assume also that $|f''(x)|$ is bounded by a constant C. Show that $f'(x_0) = y_h + O(h)$. Here we use Taylor's Theorem.

Proof: Expand $f(x_0 + h)$ using Taylor's Theorem with center of expansion x_0 we get

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(\xi) \text{ where } \xi \text{ is between } x_0 \text{ and } x_0 + h.$$

It follows then that $y_h = \dfrac{f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(\xi) - f(x_0)}{h} = f'(x_0) + \frac{h}{2} f''(\xi)$.

So $y_h = f'(x_0) + \frac{h}{2} f''(\xi)$. Using that $|f''(x)| \le C$ we get that $|f'(x_0) - y_h| \le \frac{h}{2} C$. It then follows that $f'(x_0) = y_h + O(h)$.

> $\frac{f(x_0 + h) - f(x_0)}{h}$ is called the **Forward Difference Approximation** to **f '(x)** at **x = x_0**.

Backward Difference Approximation

Given **y = f(x)** and $Y_h = \frac{f(x_0) - f(x_0 - h)}{h}$ for h > 0 and some fixed value x_0. Assume also that $|f''(x)|$ is bounded by a constant C. Show that $f'(x_0) = Y_h + O(h)$. Here we use Taylor's Theorem.

The proof is similar to that for the forward difference approximation. To start, expand $f(x_0 - h)$ using Taylor's Theorem with center of expansion x_0 and in this case ξ is between $x_0 - h$ and x_0 .

> $\frac{f(x_0) - f(x_0 - h)}{h}$ is called the **Backward Difference Approximation** to **f '(x)** at **x = x_0**.

Centered Difference Approximation

The forward and backward difference approximations are one-sided approximations to the derivative of $y = f(x)$ at $x = x_0$. A two-sided approximation to the derivative of $f(x)$ at $x = x_i$ is given by

$\mathcal{Y}_h = \frac{f(x_i + h) - f(x_i - h)}{2h}$. (This often called a *centered difference approximation* to the derivative.)

Show that $f'(x_i) = \mathcal{Y}_h + O(h^2)$. (Assume that f is three times continuously differentiable in the interval $[x_i - h, x_i + h]$.)

Proof: We use Taylor polynomial of degree two with center of expansion x_i whose error term contains f'''. We have

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

We generate expressions for $f(x_i + h)$ and $f(x_i - h)$ and manipulate them. It will be convenient to set $x = x_{i+1} = x_i + h$ and then $x = x_{i-1} = x_i - h$. Using this notation we get

$$f(x_{i+1}) = f(x_i) + f'(x_i)(h) + \frac{f''(x_i)}{2!}(h)^2 + \frac{f'''(\xi_{x_{i+1}})}{3!}(h)^3$$

and

$$f(x_{i-1}) = f(x_i) + f'(x_i)(-h) + \frac{f''(x_i)}{2!}(-h)^2 + \frac{f'''(\xi_{x_{i-1}})}{3!}(-h)^3$$

$$= f(x_i) - f'(x_i)(h) + \frac{f''(x_i)}{2!}(h)^2 - \frac{f'''(\xi_{x_{i-1}})}{3!}(h)^3$$

Then we get

$$\frac{f(x_{i+1})-f(x_{i-1})}{2h} = \frac{f(x_i)+f'(x_i)(h)+\frac{f''(x_i)}{2!}(h)^2+\frac{f'''(\xi_{x_{i+1}})}{3!}(h)^3 - \left(f(x_i)-f'(x_i)(h)+\frac{f''(x_i)}{2!}(h)^2-\frac{f'''(\xi_{x_{i-1}})}{3!}(h)^3\right)}{2h}$$

$$= \frac{2f'(x_i)(h)+\frac{f'''(\xi_{x_{i+1}})}{3!}(h)^3+\frac{f'''(\xi_{x_{i-1}})}{3!}(h)^3}{2h}$$

$$= f'(x_i)+\left(\frac{h^2}{3!}\right)\left(\frac{1}{2}f'''(\xi_{x_{i+1}})+\frac{1}{2}f'''(\xi_{x_{i-1}})\right)$$

By the Discrete Average Theorem

$$\left(\frac{h^2}{3!}\right)\left(\frac{1}{2}f'''(\xi_{x_{i+1}})+\frac{1}{2}f'''(\xi_{x_{i-1}})\right)=\left(\frac{h^2}{3!}\right)f'''(t), \text{ where } t \text{ is in } [x_{i-1},x_{i+1}].$$

Since | f'''(x)| is continuous on $[x_{i-1}, x_{i+1}]$, it is bounded, say by K. It follows that

$$\left|\frac{f(x_{i+1})-f(x_{i-1})}{2h}-f'(x_i)\right| \le K\left(\frac{h^2}{3!}\right)$$

which implies that

$$f'(x_i)=\frac{f(x_{i+1})-f(x_{i-1})}{2h}+O(h^2).$$

$\frac{f(x_0+h)-f(x_0-h)}{2h}$ is called the **Centered Difference Approximation** to **f '(x)** at **$x = x_0$**.

Notes:

- The forward and backward difference approximations are O(h); that is, they are first order approximations. Hence we expect that if h is replaced by h/2 that the error will be approximately halved.
- The forward and backward difference approximations are exact for all functions f whose second derivative is identically zero. Namely, for polynomials of degree 1 or less.
- The centered difference approximation is $O(h^2)$; that is, a second order approximation. Hence we expect that if h is replaced by h/10 that the error will drop by a factor of about 100.
- The centered difference approximation is exact for all functions whose third derivative is identically zero. Namely all polynomials of degree 2 or less.

Example:

Define: $\mathbf{D_1(h)} = \dfrac{\mathbf{f(x_0+h)-f(x_0)}}{\mathbf{h}}$ (forward difference approximation) and

$$\mathbf{D_2(h)} = \frac{\mathbf{f(x_0+h)-f(x_0-h)}}{\mathbf{2h}}$$ (centered difference approximation)

Also let $\mathbf{E_1(h) = f'(x_0) - D_1(h)}$ and $\mathbf{E_2(h) = f'(x_0) - D_2(h)}$.

Since $E_2(h)$ is $O(h^2)$ we expect E_2 to decrease by a factor of about FOUR when h is replaced by h/2;

$$\mathbf{E_2(h/2)} \approx \frac{1}{4}\mathbf{E_2(h)} \quad \text{while} \quad \mathbf{E_1(h/2)} \approx \frac{1}{2}\mathbf{E_1(h)}.$$

Thus we say E_2 decreases about twice as fast as E_1.

f(x) = e^x at x = 1

k	$D_1(h^{-k})$	$E_1(h^{-k})$	$D_2(h^{-k})$	$E_2(h^{-k})$
2	3.5268	-0.80853	2.833	-0.11469
4	3.0882	-0.36996	2.7467	-0.028404
8	2.8955	-0.1772	2.7254	-0.0070844
16	2.805	-0.086744	2.7201	-0.0017701
32	2.7612	-0.042919	2.7187	-0.00044245
64	2.7396	-0.021348	2.7184	-0.00011061
128	2.7289	-0.010646	2.7183	-2.7652e-005

Table 1.

The MATLAB code.

```
D1='(exp(1+h)-exp(1))/h';
D2='(exp(1+h)-exp(1-h))/(2*h)';
for jj=1:7,h=2^(-jj);v1(jj)=eval(D1);v2(jj)=eval(D2);end
E1=exp(1)-v1;E2=exp(1)-v2;
hv=[2 4 8 16 32 64 128]';
[hv v1' E1' v2' E2']
```

However as h gets small we expect the ***"pitfalls of computation"*** to "intrude on the computation" for obtaining $D_1(h)$ and $D_2(h)$. That is, as $\mathbf{h} \to 0$ we expect the accuracy of the approximation to deteriorate. **(WHY?)** One way to illustrate this is to use the centered difference approximation and compute the ratio of the errors at successive values of h. See Table 2.

$f(x) = e^x$ at $x = 1$

k	$D_2(h^{-k})$	$E_2(h^{-k})$	$E_2(h^{-k})/ E_2(h^{-(k+1)})$
2	2.83296779963794	-0.114685971178891	nan
4	2.74668588169833	-0.0284040532392877	4.03766216788596
8	2.72536621980373	-0.0070843913446863	4.00938511966768
16	2.72005188887067	-0.00177006041162553	4.00234438223517
32	2.71872427874553	-0.000442450286487706	4.00058597696199
64	2.71839243697998	-0.000110608520937028	4.00014648726389
128	2.7183094803361	-2.76518770574441e-005	4.00003662345414
256	2.71828874141249	-6.91295344790177e-006	4.00000915178114
512	2.71828355669641	-1.72823736033223e-006	4.0000023183001
1024	2.71828226051821	-4.32059162669418e-007	4.00000164249394
2048	2.71828193647343	-1.0801438588004e-007	4.00001499012605
4096	2.71828185546292	-2.70038738037215e-008	3.99995891941822
8192	2.71828183521029	-6.75124578464192e-009	3.99983568442305
16384	2.71828183014804	-1.68899827457381e-009	3.99718927264476
32768	2.71828182887839	-4.19343670898797e-010	4.02771853204247
65536	2.71828182855097	-9.19255782605433e-011	4.56177354370574
131072	2.71828182847821	-1.9166002118709e-011	4.79628342369897
262144	2.71828182850732	-4.82698325754427e-011	0.397059635306457
524288	2.71828182844911	9.9378283380247e-012	-4.85718116006792
1048576	2.71828182833269	1.2635315016496e-010	0.0786512115056129

TABLE 2.

The MATLAB code.

```
for jj=1:20,h=2^(-jj);k(jj)=2^jj;v2(jj)=eval(D2);end
E2=exp(1)-v2;
for jj=1:19,R2(jj)=E2(jj)/E2(jj+1);end
R2=[nan R2];
[k' v2' E2' R2']
```

Explanation:

We have the following situation:

$$\text{Total ERROR in approximating } f'(x_0) \text{ by } D_2(h) = \text{Mathematical ERROR} + \text{Roundoff ERROR}$$

the Mathematical error is incurred since $\mathbf{D_2(h)}$ is a $\mathbf{O(h^2)}$ approximation to $\mathbf{f'(x_0)}$ and the roundoff is incurred from the nature of the formula for $\mathbf{D_2(h)}$.

Let

$$f(x_0) = \text{true value of } f \text{ at } x_0 \qquad \text{Roundoff error}: \varepsilon(x^*) = f(x^*) - \tilde{f}(x^*)$$

$$f'(x_0) = \text{true value of } f' \text{ at } x_0$$

$$\tilde{f}(x_0) = \text{computed value of } f \text{ at } x_0 \text{ (for example in a floating point system)}$$

When we compute the derivative approximation **$D_2(h)$** we really get $\tilde{D}_2(h) = \dfrac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h}$

We want to measure the size of **ERROR** $= f'(x_0) - \tilde{D}_2(h)$.

$$\text{ERROR} = f'(x_0) - \tilde{D}_2(h) = f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h}$$

$$= f'(x_0) - D_2(h) + D_2(h) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h}$$

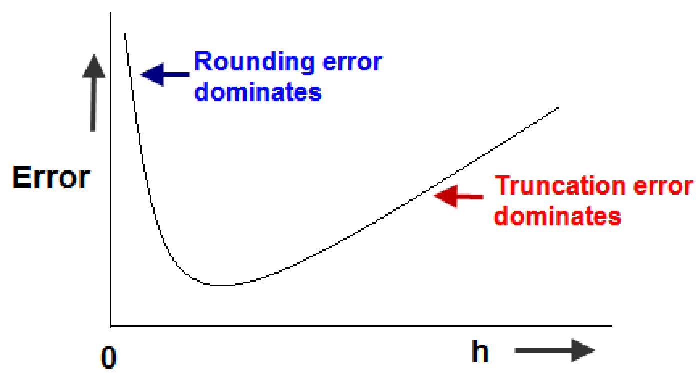
$$= -\frac{1}{6} f'''(\eta) h^2 + \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h}$$

$$= -\frac{1}{6} f'''(\eta) h^2 + \frac{f(x_0+h) - \tilde{f}(x_0+h)}{2h} - \frac{f(x_0-h) - \tilde{f}(x_0-h)}{2h}$$

$$= -\frac{1}{6} f'''(\eta) h^2 + \frac{\varepsilon(x_0+h) - \varepsilon(x_0-h)}{2h}$$

MATH ERROR **Roundoff error**

(Truncation Error)



We can **delay the effects** of 'Roundoff Error' by using more digits in a computation, but cannot eliminate it.

Other Derivative Approximations

- A second order forward difference first derivative approximation:

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{h^2}{3} f'''(\xi)$$

- A second order backward difference first derivative approximation:

$$f'(x_0) = \frac{3f(x_0) - 4f(x_0-h) + f(x_0-2h)}{2h} + \frac{h^2}{3} f'''(\xi)$$

- A second order central difference second derivative approximation:

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi)$$

Example:

Let **f(x) = xe^x**. Then $\mathbf{f'(x) = (x+1)e^x}$ and $\mathbf{f'(2.0) \approx 22.167168}$. We want to approximate $\mathbf{f'(2)}$ using several first order formulas and several second order formula employing the data in the table.

x	f(x)
1.8	10.889365
1.9	12.703199
2	14.778112
2.1	17.148957
2.2	19.855030

Forward Difference approximation:

$$\frac{\mathbf{f}(2+0.1) - \mathbf{f}(2)}{0.1} = 23.70845 \quad \textbf{Abs.Error} \approx 1.541282$$

Backward Difference approximation:

$$\frac{\mathbf{f}(2) - \mathbf{f}(2-0.1)}{0.1} = 20.74913 \quad \textbf{Abs.Error} \approx 1.418038$$

Centered Difference approximation:

$$\frac{\mathbf{f}(2+0.1) - \mathbf{f}(2-0.1)}{2(0.1)} = 22.22879 \quad \textbf{Abs.Error} \approx 0.061622$$

Using 3-point forward difference formula:

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{h^2}{3} f'''(\xi)$$

$$\frac{\mathbf{-3f(2) + 4f(2.1) - f(2.2)}}{\mathbf{2(0.1)}} = \mathbf{22.03231} \quad \textbf{Abs. Error} \approx \mathbf{0.134858}$$

Using 3-point backward difference formula:

$$f'(x_0) = \frac{3f(x_0) - 4f(x_0-h) + f(x_0-2h)}{2h} + \frac{h^2}{3} f'''(\xi)$$

$$\frac{\mathbf{3f(2) - 4f(1.9) + f(1.8)}}{\mathbf{2(0.1)}} = \mathbf{22.054525} \quad \textbf{Abs. Error} \approx \mathbf{0.107155}$$