Error Analysis of Finite Difference Derivative Formulas

Answers

1. $\frac{d^2f}{dx^2}$ or $f''(x)$ is being approximated.
2. From the above calculation, the leading order truncation error is $\frac{h^2}{12}f''''(x)$
3. $\frac{4\epsilon f(x)}{h^2}$
4. $h = \sqrt[4]{\left|\frac{48\epsilon_{mach}f(x)}{f^{(4)}(x)}\right|}$
5. $2\sqrt{\left|\frac{\epsilon_{mach}f(x)f^{(4)}(x)}{3}\right|}$

Working out the answers:

Part 1&2

$$g(x,h) = (f(x+h) + f(x-h) - 2f(x))/h^2$$

From taylors expansion we know that

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f''''(x) + \frac{h^5}{5!}f'''''(x) + O(h^6)$$

Therefore, by substitution (with $h = h$ and $h = -h$) and simple rearrangement,

$$h^2g(x,h) = hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + -hf(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f''''(x) + \frac{h^5}{5!}f'''''(x) + \frac{h^4}{4!}f''''(x) - \frac{h^5}{5!}f'''''(x) + O(h^6)$$

$$\Rightarrow h^2g(x,h) = h^2f''(x) + \frac{h^4}{12}f''''(x) + O(h^6)$$

$$\Rightarrow g(x,h) = f''(x) + \frac{h^2}{12}f''''(x) + O(h^4)$$

Under suitable assumptions of smoothness,

$$\lim_{h\to 0} g(x,h) = f''(x)$$

Thus, the truncation error is $\frac{h^2}{12}f^{(4)}(x)$

Part 3

We'll use $\widehat{w}$ to represent the floating point version of w.

$$\hat{g} = \frac{\left(\hat{f}(\hat{x}+\hat{h}) + \hat{f}(\hat{x}-\hat{h}) - 2\hat{f}(\hat{x})\right)}{\widehat{h^2}}$$

We also know that $\hat{f}(\widehat{w}) = f(\widehat{w})(1+\epsilon)$ for some $\epsilon \leq \epsilon_{mach}$

Let $f_0 \equiv f(\hat{x})$, $f_1 \equiv f(\hat{x}+\hat{h})$, $f_2 \equiv f(\hat{x}-\hat{h})$.

Thus, $\widehat{f_0} = f_0(1+\epsilon_0)$, $\widehat{f_1} = f_1(1+\epsilon_1)$, $\widehat{f_2} = f_2(1+\epsilon_2)$

Thus, $\hat{g} = \frac{\widehat{f_1}+\widehat{f_2}-2\widehat{f_0}}{\widehat{h^2}} = \frac{f_1+f_2-2f_0}{\widehat{h^2}} + \frac{f_1\epsilon_1+f_2\epsilon_2-2f_0\epsilon_0}{\widehat{h^2}}$

1. The first term is the derivative that we want to compute.
2. Under limit $h \to 0$, $f_0 = f_1 = f_2$.

$$\therefore \hat{g} = (f''(\hat{x}) + truncation\ error) + \frac{f_0(\epsilon_1+\epsilon_2-2\epsilon_0)}{h^2}$$

We can bound the second term, which is the round off error by $\frac{4\epsilon_{mach}f(x)}{h^2}$

Part 4

We now know that the total error is $error = \frac{4\epsilon_{mach}f(x)}{h^2} + \frac{h^2}{12}f^{(4)}(x)$

To minimize wrt h, we look at the first differential wrt h:

$$\frac{d(error)}{dh} = -\frac{8\epsilon_{mach}f(x)}{h^3} + \frac{hf^{(4)}(x)}{6} = 0$$

$$\Rightarrow \frac{-48\epsilon_{mach}f(x) + h^4f^{(4)}(x)}{6h^3} = 0$$

Alas! We are forced to deal with this *terrifying* equation. But we are brave, and hopefully not stupid, so lets carry on.

Let

$$a = |f^{(4)}(x)|$$

$$b = |48\epsilon_{mach}f(x)|$$

$$\therefore h^4a - b = 0$$

$$\Rightarrow \left(h^2\sqrt{a} - \sqrt{b}\,\right)\left(h^2\sqrt{a} + \sqrt{b}\,\right) = 0$$

$$\Rightarrow \left(h\sqrt[4]{a} + \sqrt[4]{b}\right)\left(h\sqrt[4]{a} - \sqrt[4]{b}\right)\left(h^2\sqrt{a} + \sqrt{b}\,\right) = 0$$

For this to be a minimizer, we must look at the second derivative of error. It is

$$\frac{|h^4f^{(4)}| - 144|\epsilon_{mach}f|}{6h^4} = \frac{h^4a - 3b}{6h^4}$$

If the second derivative is positive, we're good. Since h must be real, we have two possibilities - $\pm\sqrt[4]{b/a}$, we have that the second derivative at both values is $-\frac{b}{3h^4}$.

Notice that $g(x,h)$ is symmetric wrt h, hence we'll only talk about $+\sqrt[4]{b/a}$ and ignore $-\sqrt[4]{b/a}$.

$$h = \sqrt[4]{|\frac{48\epsilon_{mach}f(x)}{f^{(4)}(x)}|}$$

is the minimizer.

Part 5

Substituting the value of h into error, we get that total error is

$$2\sqrt{|\frac{\epsilon_{mach}f(x)f^{(4)}(x)}{3}|}$$