Introduction to Numerical Analysis I
Handout 9

1 Numerical Differentiation and Integration

We developed a tool (interpolation) which will serve us in future as following: Given $P_n(x)$ is a polynomial interpolation of $f(x)$, for each linear operator L we have

$$Lf(x) \approx LP_n(x)$$

and the error given by

$$e(x) = L[f(x) - P_n(x)] = Lf\{[x_0, \ldots, x_n, x]\, p(x)\}$$

where $p(x) = \prod_{k=0}^{n}(x - x_k)$.

1.1 Numerical Differentiation/Finite Differences

Definition 1.1 (First Numerical Derivative). Let $P_n(x)$ be polynomial interpolation of $f(x)$ at interpolation points $\{x_k\}_{k=0}^n$, then

$$f'(x) = P_n'(x) + \frac{d}{dx}\{f[x_0, \ldots, x_n, x]\, p(x)\}$$

The error is given by

$$e(x) = f'(x) - P_n'(x) = \frac{d}{dx}\{f[x_0, \ldots, x_n, x]\, p(x)\} =$$
$$= f[x_0, \ldots, x_n, x]\, p'(x) + p(x)\frac{d}{dx}f[x_0, \ldots, x_n, x]$$

From the term $\frac{d}{dx}f[x_0, \ldots, x_n, x]$ we learn that we need to differentiate divided differences.

Definition 1.2 (Derivative of DD).

$$\frac{d}{dx}f[x_0, \ldots, x_k, x] =$$
$$\lim_{h\to 0}\frac{f[x_0, \ldots, x_k, x+h] - f[x_0, \ldots, x_k, x]}{h} =$$
$$\lim_{h\to 0} f[x_0, \ldots, x_k, x, x+h] = f[x_0, \ldots, x_k, x, x]$$

Finally, given that $f(x)$ have $n+2$ derivatives, the error formula is

$$e(x) = f'(x) - P_n'(x) =$$
$$f[x_0, \ldots, x_n, x]\, p'(x) + p(x)\, f[x_0, \ldots, x_n, x, x] =$$
$$= \frac{f^{(n+1)}(c)}{(n+1)!}p'(x) + \frac{f^{(n+2)}(\tilde{c})}{(n+2)!}p(x)$$

Note that in the simplest case, one of the polynomial parts $p(x)$ or $p'(x)$ vanishes.

Example 1.3.

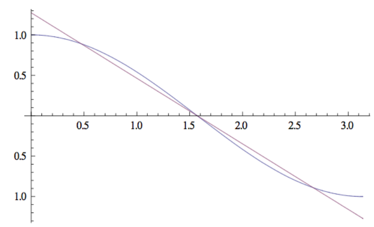
$$f(x) \approx P_2(x) = f[a] + f[a, a+h](x-a)$$

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

Thus,

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

Example 1.4. We previously found $\sin x \approx P_3(x) = \frac{4}{\pi}x - \frac{4}{\pi^2}x^2$, therefore $\cos x \sin' x \approx \frac{d}{dx}P_3(x) = \frac{4}{\pi} - \frac{8}{\pi^2}x \approx 1.27 - 0.81x$



Definition 1.5 (Higher order Numerical Differentiation). Let $P_n(x)$ be polynomial interpolation of $f(x)$ at interpolation points $\{x_k\}_{k=0}^n$. Suppose that $f(x)$ have $n+m+1$ derivatives ($m \le n$), then

$$f^{(m)}(x) = P_n^{(m)}(x) + \frac{d^m}{dx^m}\{f[x_0, \ldots, x_k, x]\, p(x)\}$$

And the error is given by

$$e(x) = f^{(m)}(x) - P_n^{(m)}(x) = \frac{d^m}{dx^m}\{f[x_0, \ldots, x_k, x]\, p(x)\} =$$
$$\frac{d^{m-1}}{dx^{m-1}}\{f[x_0, \ldots, x_n, x]\, p'(x) + f[x_0, \ldots, x_n, x, x]\, p(x)\} =$$
$$\frac{d^{m-2}}{dx^{m-2}}\{f[x_0, \ldots, x_n, x]\, p''(x) + 2f[x_0, \ldots, x_n, x, x]\, p'(x) + f[x_0, \ldots, x_n, x, x, x]\, p(x)\} = \cdots$$

Definition 1.6 (Forward (Backward) Differences:). (partially) uses interpolation points $\{a + jh\}_{j=0}^n$ $\left(\{a - jh\}_{j=0}^n\right)$

Definition 1.7 (Central Differences:). (partially) uses interpolation points $\{a + jh\}_{j=0}^n \cup \{a - jh\}_{j=0}^n$ symmetrically.

Theorem 1.8. Let m be an integer and let $n + 1 = 2m$. Given interpolation points $x_0 \le \ldots \le x_n$ symmetrically distributed around a point a, that is $a - x_{(m-1)-k} = -(a - x_{m+k})$ or alternatively

$$a = \frac{x_{(m-1)-k} + x_{m+k}}{2}$$

for any k, then $\frac{d}{dx}\prod_{k=0}^{n}(x - x_k)\Big|_{x=a} = 0$.

1.1.1 Developing FD schemes using Polynomial Basis

Definition 1.9 (**The order of approximation).** The order of approximation is defined to be the minimal p that satisfies the following inequality

$$|e(x)| \leq ch^p = O(h^p),$$

where $e(x)$ is the error of approximation and

$$\min_{i \neq j} |x_i - x_j| \leqslant h \leqslant \max_{i \neq j} |x_i - x_j| .$$

Example 1.10. For example the central difference formula for the first derivative has a first order, that is of second order, since

$$f'(a) = \frac{f(a+h) - f(a-h)}{2h} + O(h^2)$$

Definition 1.11 (**Algebraic Order of Exactness).** An approximation method has an algebraic order of exactness p if p is the maximal degree of a polynomial for which the approximation provides an exact solution.

Example 1.12. For example consider Polynomial basis $\{1, x, x^2, x^3, ...\}$ The forward formula gives a first order

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

$$f = 1 \Rightarrow \frac{1-1}{h} = 0 = f'$$

$$f = x \Rightarrow \frac{x+h-x}{h} = 1 = f'$$

$$f = x^2 \Rightarrow \frac{(x+h)^2 - x^2}{h} = \frac{2xh + h^2}{h} = 2x + O(h)$$

The latest example provide an algorithm to create FD schemes. Let D be differential operator. To approximate D at point a by $\mathcal{D}f(a) = \sum_{j=1}^{p} c_j f(a+jh)$ one solves the following linear system of equation

$$\begin{pmatrix} \mathcal{D}\,1 \\ \mathcal{D}\,x \\ \vdots \\ \mathcal{D}\,x^p \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_p \end{pmatrix} = \begin{pmatrix} D\,1 \\ D\,x \\ \vdots \\ D\,x^p \end{pmatrix}$$

Example 1.13. Let $f'(a) \approx c_1 f(a) + c_2 f(a-h)$. To find c_1, c_2 solve

$$f = 1 \Rightarrow c_1 + c_2 = 0 \Rightarrow c_2 = -c_1$$
$$f = x \Rightarrow c_1 a + c_2 (a-h) = 1$$

To get the backward formula $f'(a) \approx \frac{f(a)-f(a-h)}{h}$

1.1.2 Developing FD schemes using Taylor Expansion

Consider $f'(a) \approx c_1 f(a) + c_2 f(a-h) + c_3 f(a+h)$

The Taylor expansion gives

$f(a) = f(a)$

$f(a \pm h) = f(a) \pm hf'(a) + \frac{h^2}{2} f''(a) \pm \frac{h^3}{6} f^{(3)}(a) + \mathcal{O}\left(h^4\right)$

Rewrite in the matrix form

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} f(a) \\ hf'(a) \\ \frac{h^2}{2} f''(a) \end{bmatrix} = \begin{bmatrix} f(a) \\ f(a+h) \\ f(a-h) \end{bmatrix} + O\left(h^3\right)$$

We don't need to solve the linear system. One writes

$$f(a \pm h) - f(a) = \pm hf'(a) + \frac{h^2}{2} f''(a) + \mathcal{O}\left(h^3\right)$$

Subtract between the $(\pm)$ equations to get $f(a+h) - f(a-h) = 2hf'(a) + \mathcal{O}\left(h^3\right)$ then solve for $f'(a)$ to get the central formula. Similarly, add between the equations to get

$$f(a+h) - 2f(a) + f(a-h) = h^2 f''(a) + \mathcal{O}\left(h^4\right)$$

$$\Rightarrow f''(a) = \frac{f(a+h) - 2f(a) + f(a-h)}{h^2} + \mathcal{O}\left(h^2\right)$$

1.1.3 Sensitivity to error

Let $\tilde{f}(x) = f(x) + \tilde{e}(x)$ and assume $|\tilde{e}(x_j)| \leqslant \varepsilon$ and $\left|f^3(x)\right| \leqslant M$. Use the central formula for first derivative $f'(a) = \frac{f(a+h)-f(a-h)}{2h} - \frac{f^{(3)}(c)}{6} h^2$.

Then

$$\tilde{f}'(a) = \frac{f(a+h) - f(a-h)}{2h} - \frac{f^{(3)}(c)}{6} h^2 + \frac{\tilde{e}(a+h) - \tilde{e}(a-h)}{2h}$$

Thus, the error is

$$e(x) = \left| -\frac{f^{(3)}(c)}{6} h^2 + \frac{\tilde{e}(a+h) - \tilde{e}(a-h)}{2h} \right| \leqslant \left| \frac{M}{6} h^2 \right| + \frac{|\tilde{e}(a+h)| + |\tilde{e}(a-h)|}{2h} = \left| \frac{M}{6} h^2 \right| + \frac{\varepsilon}{h} \underset{h \to 0}{\to} \infty$$

To find the optimal value of h one solves

$$e'(x) = \frac{M}{3} h - \frac{\varepsilon}{h^2} = 0$$

to get $h = \sqrt[3]{\frac{3}{M} \varepsilon}$. See the graph of $e(x)$ below.