Department of Mathematics, University of Utah

Analysis of Numerical Methods I
MTH6610 – Section 001 – Fall 2019

Lecture notes – Numerical differentiation
Friday, November 22, 2019

These notes are not a substitute for class attendance. Their main purpose is to provide a lecture overview summarizing the topics covered.

We seek to develop approximate formulas for computing derivatives of functions. Our approximations will take a form similar to quadrature formulas:

$$f'(x) \approx \sum_{j=1}^{N} w_j f(x_j), \qquad x, x_1, \ldots, x_N \in [a,b]. \tag{1}$$

Formulas of the above type are called *finite difference* formulas. (We will see that some weights are negative so that the above is a subtraction, or difference, of evaluations.) In order to introduce the basic idea, we simplify the above task to a special case: suppose we wish to approximate $f'(x)$ using the points $x_1 = x$ and $x_2 = x + h$. Thus we are looking for a formula of the form

$$f'(x) \approx w_1 f(x) + w_2 f(x+h),$$

where the weights w_1 and w_2 must be computed. In order to accomplish this, we require Taylor's Theorem. Recall the following formula, which is Taylor's Theorem in Lagrange form: If f has $(p+1)$ continuous derivatives on $[a,b]$, then

$$f(y) = \sum_{j=0}^{p} \frac{f^{(j)}(x)}{j!}(y-x)^j + \frac{f^{(p+1)}(\xi)}{(p+1)!}(\xi - x)^{p+1}, \qquad \xi = \xi(y) \in [x,y],$$

where we have the convention $f^{(0)} = f$ and $0! = 1$. Applying this formula with $p = 1$ to $y = x + h$, we have

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi) = f(x) + hf'(x) + \mathcal{O}(h^2),$$

where the statement $\mathcal{O}(h^2)$ assumes that f'' is bounded. If we linearly combine this expression with $f(x)$, then we obtain

$$f(x+h) - f(x) = hf'(x) + \mathcal{O}(h^2) \quad \Longrightarrow \quad -\frac{1}{h} f(x) + \frac{1}{h} f(x+h) = f'(x) + \mathcal{O}(h),$$

showing that $w_1 = -1/h$ and $w_2 = 1/h$ achieves our desired goal, with the error decaying like h as $h \to 0$. Thus this is a *first order* approximation to the derivative.
We can now generalize this to the case (1): since

$$f(x_j) = \sum_{k=0}^{N-1} \frac{f^{(k)}(x)}{k!}(x_j - x)^k + \mathcal{O}((b-a)^N),$$

---

then by matching $f(x)$, $f'(x)$, …, $f^{(N-1}(x)$ terms, we want the w_j to satisfy the linear system

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ (x_1 - x) & (x_2 - x) & (x_3 - x) & \cdots & (x_N - x) \\ \frac{(x_1-x)^2}{2} & \frac{(x_2-x)^2}{2} & \frac{(x_3-x)^2}{2} & \cdots & \frac{(x_N-x)^2}{2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{(x_1-x)^{N-1}}{(N-1)!} & \frac{(x_2-x)^{N-1}}{(N-1)!} & \frac{(x_3-x)^{N-1}}{(N-1)!} & \cdots & \frac{(x_N-x)^{N-1}}{(N_1)!} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_N \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

The solution vector $\boldsymbol{w} \in \mathbb{R}^N$ to this system contains the weights w_j for the formula (1). Note in general that once we find weights such that (1) holds, the error will behave like

$$f'(x) = \sum_{j=1}^{N} w_j f(x_j) + \mathcal{O}((b-a)^{N-1}),$$

where we will have order $N-1$ instead of N for the same reason as in our derivation of the $N = 2$ case. Since we usually assume that the interval $[a, b]$ is small, then this results in order $N-1$ convergence as $(b-a) \to 0$.
However, sometimes one obtains a higher-order estimate than expected. Consider $N = 2$ with

$$x_1 = x - h, \qquad\qquad x_2 = x + h,$$

and we wish to compute a numerical differentiation formula for $f'(x)$. The same computations as above yields

$$w_1 = -\frac{1}{2h}, \qquad\qquad w_2 = \frac{1}{2h}.$$

We expect an order of convergence of $(N-1) = 1$. Yet when we use Taylor's Theorem, we see that

$$f(x \pm h) = f(x) \pm hf'(x) + \frac{h^2}{2} f''(x) + \mathcal{O}(h^3),$$

so that

$$-\frac{1}{2h} f(x-h) + \frac{1}{2h} f(x+h) = 0f''(x) + \mathcal{O}(h^2) = \mathcal{O}(h^2).$$

Thus, we obtain order-2 convergence for this special configuration of nodes in the differentiation formula.