Notes for section 4.1

Math. 481a,Spring 2026

Numerical differentiation

We want to approximate $f'(x_0)$ for some $x_0 \in (a,b)$ and $f \in C^2[a,b]$. We start with h small enough that $x_1 = x_0 + h \in [a,b]$. If $P_{0,1}(x)$ is the Lagrange polynomial interpolating f at x_0 and x_1, we have

$$\begin{aligned} f(x) &= P_{0,1}(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)) \\ &= \frac{(x-x_0-h)f(x_0)}{-h} + \frac{(x-x_0)f(x_0+h)}{h} + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)), \qquad \text{for some } \xi(x) \in [a,b]. \end{aligned} \tag{1}$$

After differentiating both sides of (1) with respect to x we obtain

$$\begin{aligned} f'(x) &= \frac{f(x_0+h)-f(x_0)}{h} + D_x\left[\frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))\right] \\ &= \frac{f(x_0+h)-f(x_0)}{h} + \frac{2(x-x_0)-h}{2} f''(\xi(x)) + \frac{(x-x_0)(x-x_1)}{2!} \cdot D_x\left(f''(\xi(x))\right). \end{aligned}$$

For arbitrary x we don't have any information about the magnitude of $D_x\left(f''(\xi(x))\right)$, however, when $x = x_0$, the above equation reduces itself to

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

For $h > 0$ the above formula is called **Two-Point Forward-Difference Formula**, while for $h < 0$ it is called **Two-Point Backward-Difference Formula**.

In general, we suppose that $x_0, x_1, \dots, x_n \in [a,b]$ are distinct and $f \in C^{n+1}[a,b]$. The Lagrange interpolation theorem implies that

$$f(x) = \sum_{k=0}^{n} f(x_k) L_{n,k}(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n), \tag{2}$$

where

$$L_{n,k}(x) = \frac{(x-x_0)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_n)}{(x_k-x_0)\cdots(x_k-x_{k-1})(x_k-x_{k+1})\cdots(x_k-x_n)} = \prod_{\substack{i=0 \\ i\neq k}}^{n} \frac{(x-x_i)}{(x_k-x_i)},$$

and $\xi(x) \in [a,b]$.

Differentiating both sides of (2) with respect to x we obtain

$$\begin{aligned} f'(x) &= \sum_{k=0}^{n} f(x_k) L'_{n,k}(x) \\ &\quad + D_x\left[\frac{(x-x_0)(x-x_1)\cdots(x-x_n)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) + \frac{(x-x_0)(x-x_1)\cdots(x-x_n)}{(n+1)!} D_x\left[f^{(n+1)}(\xi(x))\right]. \end{aligned}$$

As before we have a problem with determining the size of $D_x\left[f^{(n+1)}(\xi(x))\right]$. However, when $x = x_j$, we obtain

$$f'(x_j) = \sum_{k=0}^{n} f(x_k) L'_{n,k}(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0 \\ k\neq j}}^{n} (x_j - x_k). \tag{3}$$

The above formula is called **(n+1)-point formula** to approximate $f'(x_j)$.

In general using more nodal (evaluation) points results in greater accuracy, although the number of functional evaluations and growth of round-off error has to be taken into account.

Derivation of three-point formulas

For x_0, x_1, x_2, formula (3) becomes

$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right] + f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right]$$
$$+ \frac{1}{6} f^{(3)}(\xi_j) \prod_{\substack{k=0 \\ k \neq j}}^{2} (x_j - x_k).$$

When the points are equally spaced,

$$x_1 = x_0 + h, \qquad x_2 = x_0 + 2h,$$

the above formula becomes much simpler.

For $x_j = x_0$, $x_1 = x_0 + h$, and $x_2 = x_0 + 2h$, we obtain

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0 + h) - \frac{1}{2}f(x_0 + 2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0).$$

For $x_j = x_1$, $x_1 = x_0 + h$, and $x_2 = x_0 + 2h$, we obtain

$$f'(x_0 + h) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0 + 2h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1).$$

For $x_j = x_2$, $x_1 = x_0 + h$, and $x_2 = x_0 + 2h$, we obtain

$$f'(x_0 + 2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0 + h) + \frac{3}{2}f(x_0 + 2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_2).$$

Finally, substituting x_0 for $x_0 + h$ in the second formula above, and substituting x_0 for $x_0 + 2h$ in the third formula above, we have

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0),$$
$$f'(x_0) = \frac{1}{2h}\left[-f(x_0 - h) + f(x_0 + h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1)$$
$$f'(x_0) = \frac{1}{2h}\left[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)\right] + \frac{h^2}{3} f^{(3)}(\xi_2).$$

Finally, since the last of above formulas can be obtained from the first by replacing h with $-h$, there are only two formulas

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0), \tag{4}$$

where ξ_0 lies between x_0 and $x_0 + 2h$ and

$$f'(x_0) = \frac{1}{2h}\left[f(x_0 + h) - f(x_0 - h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1), \tag{5}$$

where ξ_1 lies between $x_0 - h$ and $x_0 + h$.

The errors in both (4) and (5) are of order $O(h^2)$, however, the error in (5) is approximately half the error in (4). This is due the fact that (5) uses data on both sides of x_0. Additionally, f needs to be evaluated at only two points.

Five-Point Formulas

Here is an example of one of the **Five-Point Formulas**:

$$f'(x_0) = \frac{1}{12h}\left[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)\right] + \frac{h^4}{30} f^{(5)}(\xi).$$

Approximation of higher order derivatives

Expanding f in Taylor polynomial about x_0 and evaluating it at x_0+h and x_0-h we have:

$$f(x_0+h)=f(x_0)+f'(x_0)h+\frac{1}{2}f''(x_0)h^2+\frac{1}{6}f'''(x_0)h^3+\frac{1}{24}f^{(4)}(\xi_1)h^4$$

and

$$f(x_0-h)=f(x_0)-f'(x_0)h+\frac{1}{2}f''(x_0)h^2-\frac{1}{6}f'''(x_0)h^3+\frac{1}{24}f^{(4)}(\xi_{-1})h^4$$

Adding the above two equations and solving for $f''(x_0)$ we get

$$f''(x_0)=\frac{1}{h^2}\left[f(x_0-h)-2f(x_0)+f(x_0+h)\right]-\frac{h^2}{24}\left[f^{(4)}(\xi_1)+f^{(4)}(\xi_{-1})\right]. \quad (6)$$

When $f^{(4)}$ is continuous on $[x_0-h,x_0+h]$ and since $\frac{1}{2}\left[f^{(4)}(\xi_1)+f^{(4)}(\xi_{-1})\right]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the Intermediate Value Theorem implies that there exists ξ between ξ_1 and ξ_{-1}, with

$$f^{(4)}(\xi)=\frac{1}{2}\left[f^{(4)}(\xi_1)+f^{(4)}(\xi_{-1})\right],$$

and (6) becomes

$$f''(x_0)=\frac{1}{h^2}\left[f(x_0-h)-2f(x_0)+f(x_0+h)\right]-\frac{h^2}{12}f^{(4)}(\xi).$$

Round-off error

Suppose that we are making round-off errors $e(x_0+h)$ and $e(x_0-h)$ in evaluating $f(x_0+h)$ and $f(x_0-h)$, respectively. Then, the computed values $f(x_0+h)=\tilde{f}(x_0+h)+e(x_0+h)$ and $f(x_0-h)=\tilde{f}(x_0-h)+e(x_0-h)$ transform formula (5) into

$$f'(x_0)-\frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}=\frac{e(x_0+h)-e(x_0-h)}{2h}-\frac{h^2}{6}f^{(3)}(\xi_1).$$

Suppose now that

$$|e(x_0\pm h)|\le\epsilon \qquad \text{and} \qquad |f^{(3)}(\xi)|\le M,$$

then

$$\left|f'(x_0)-\frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}\right|\le\frac{\epsilon}{h}+\frac{h^2}{6}M.$$

To reduce the truncation error, $h^2M/6$, we must reduce h, however, by reducing h the round-off error ϵ/h grows. In practice, it is rarely advantageous to let h to be too small since the round-off error will dominate the calculations.