## 7. Approximation of Derivatives

Basic idea: replace the function by its interpolating polynomial and use the derivative of the interpolating polynomial as an approximation to the derivative of the function.

### 7.1. **Numerical Differentiation Formulas.**

Let $P_n(x)$ be the unique polynomial of degree $\leq n$ interpolating $f$ at $x_0, \ldots, x_n$. Then $f(x) - P_n(x) = f[x_0, \ldots x_n, x]\psi_n(x)$, where $\psi_n(x) = \prod_{j=0}^{n}(x - x_j)$. If we approximate $f'(x)$ by $P_n'(x)$, then the error

$$f'(x) - P_n'(x) = \{(d/dx)f[x_0, \ldots, x_n, x]\}\psi_n(x) + f[x_0, \ldots, x_n, x]\psi_n'(x).$$

Now suppose that $f \in C^{n+2}$. Then

$$(d/dx)f[x_0, \ldots, x_n, x] = \lim_{h \to 0} \frac{f[x_0, \ldots, x_n, x+h] - f[x_0, \ldots, x_n, x]}{h}.$$

But

$$\begin{aligned} f[x_0, \ldots, x_n, x, x+h] &= f[x, x_0, \ldots, x_n, x+h] \\ &= (1/h)\{f[x_0, \ldots, x_n, x+h] - f[x, x_0, \ldots, x_n]\} \\ &= (1/h)\{f[x_0, \ldots, x_n, x+h] - f[x_0, \ldots, x_n, x]\}. \end{aligned}$$

Hence,

$$(d/dx)f[x_0, \ldots, x_n, x] = \lim_{h \to 0} f[x_0, \ldots, x_n, x, x+h] = f[x_0, \ldots, x_n, x, x].$$

Thus the error formula becomes:

$$\begin{aligned} f'(x) - P_n'(x) &= f[x_0, \ldots, x_n, x, x]\psi_n(x) + f[x_0, \ldots, x_n, x]\psi_n'(x) \\ &= f^{(n+2)}(\xi_x)\psi_n(x)/(n+2)! + f^{(n+1)}(\eta_x)\psi_n'(x)/(n+1)!, \end{aligned}$$

for some $\xi_x, \eta_x \in (a, b)$.

Next consider a special case when the error formula can be simplified: $x$ is one of the interpolation points $x_i$. Then $\psi_n(x_i) = 0$ and so

$$f'(x_i) - P_n'(x_i) = f[x_0, \ldots, x_n, x_i]\psi_n'(x_i) = f^{(n+1)}(\eta_x)\psi_n'(x_i)/(n+1)!.$$

Writing $\psi(x) = (x - x_i)\prod_{\substack{j=0 \\ j \neq i}}^{n}(x - x_j)$, we see that $\psi_n'(x_i) = \prod_{\substack{j=0 \\ j \neq i}}^{n}(x_i - x_j)$ and so

$$f'(x_i) - P_n'(x_i) = f[x_0, \ldots, x_n, x_i]\prod_{\substack{j=0 \\ j \neq i}}^{n}(x_i - x_j) = f^{(n+1)}(\eta_x)\prod_{\substack{j=0 \\ j \neq i}}^{n}(x_i - x_j)/(n+1)!.$$

Examples:

$n = 1$:

$P_1(x) = f(x_0) + f[x_0, x_1](x - x_0)$. Hence, $P_1'(x) = f[x_0, x_1]$ for all $x$. Then

$$f'(x_0) - P_1'(x_0) = -hf^{(2)}(\eta_x)/2, \qquad f'(x_1) - P_1'(x_1) = hf^{(2)}(\eta_x)/2,$$

where $h = x_1 - x_0$.

$n = 2$:

$P_2(x) = f(x_0) + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1)$. Hence, $P_2'(x) = f[x_0, x_1] + f[x_0, x_1, x_2](2x - x_0 - x_1)$. When $x = x_1$, and the points are equally spaced with $x_{i+1} - x_i = h$, we get:

$$\begin{aligned} P_2'(x_1) &= f[x_0, x_1] + f[x_0, x_1, x_2](x_1 - x_0) \\ &= f[x_0, x_1] + (f[x_1, x_2] - f[x_0, x_1])\frac{x_1 - x_0}{x_2 - x_0} \\ &= (f[x_1, x_2] + f[x_0, x_1])/2 = [f(x_2) - f(x_0)])/(2h) = f[x_0, x_2]. \end{aligned}$$

The error is given by: $f'(x_i) - P_n'(x_i) = f^{(n+1)}(\eta_x) \prod_{\substack{j=0 \\ j \neq i}}^{n} (x_i - x_j)/(n+1)!$ and so

$$\begin{aligned} f'(x_0) - P_2'(x_0) &= f^{(3)}(\eta_x)(x_0 - x_1)(x_0 - x_2)/6, \\ f'(x_1) - P_2'(x_1) &= f^{(3)}(\eta_x)(x_1 - x_0)(x_1 - x_2)/6, \\ f'(x_2) - P_2'(x_2) &= f^{(3)}(\eta_x)(x_2 - x_0)(x_2 - x_1)/6. \end{aligned}$$

If the points are equally spaced with $x_{i+1} - x_i = h$, then

$$\begin{aligned} f'(x_0) - P_2'(x_0) &= h^2 f^{(3)}(\eta_x)/3, \\ f'(x_1) - P_2'(x_1) &= -h^2 f^{(3)}(\eta_x)/6, \\ f'(x_2) - P_2'(x_2) &= h^2 f^{(3)}(\eta_x)/3. \end{aligned}$$

Note that the error formula says that the divided difference $f[x_0, x_2]$ approximates $f'(x_1)$ with error $-h^2 f^{(3)}(\eta_x)/6$. On the other hand, using the Taylor series expansion $f(x_2) = f(x_0) + f'(x_0)(x_2 - x_0) + f''(\xi)(x_2 - x_0)^2/2$, we get

$$f[x_0, x_2] - f'(x_0) = \frac{f(x_2) - f(x_0)}{x_2 - x_0} - f'(x_0) = f''(\xi)(x_2 - x_0)/2 = hf''(\xi).$$

Using a Taylor expansion about $x_2$, we get $f[x_0, x_2] - f'(x_2) = -hf''(\xi)$. Hence, $f[x_0, x_2]$ gives a higher order approximation to $f'$ at the midpoint of the interval than at the two end points.

We also obtain formulas for approximating higher derivatives in a similar way.

Example: $n = 2$. $P_2''(x) = 2f[x_0, x_1, x_2]$. Consider the case of equally spaced points: $x_0 = a - h, x_1 = a, x_2 = a + h$. Then $P_2''(x) = [f(a+h) - 2f(a) + f(a+h)]/h^2$. In this case, we can easily derive an error formula for $f''(a) - P_2''(a)$ by using Taylor series expansions.

$$f(a \pm h) = f(a) \pm f'(a)h + f''(a)h^2/2 \pm f^{(3)}(a)h^2/6 + f^{(4)}(\xi_\pm)h^4/4!.$$

Hence,

$$[f(a+h) - 2f(a) + f(a+h)]/h^2 = f''(a) + h^2[f^{(4)}(\xi_+) + f^{(4)}(\xi_-)]/4! = f''(a) + h^2 f^{(4)}(\xi)/12,$$

and so

$$f''(a) - [f(a+h) - 2f(a) + f(a+h)]/h^2 = -h^2 f^{(4)}(\xi)/12.$$

This estimate uses symmetry to get cancellations in the error. The approximation would only be $O(h)$ at other points.

7.2. **Roundoff Error in Numerical Differentiation.** Consider the formula:

$$f'(a) = [f(a+h) - f(a-h)]/(2h) - h^2 f''(\xi)/6.$$

This equation says that if $|f''(x)| \le M_2$ for all $x \in [a-h, a+h]$, then the sequence $[f(a+h) - f(a-h)]/(2h)$ converges to $f'(a)$ as $h \to 0$.

This assumes, however that the quantity $[f(a+h) - f(a-h)]/(2h)$ is computed exactly. Because of roundoff errors, we will really be using the numbers $f(a+h)+E_+$ and $f(a-h)+E_-$ in the calculations. Then

$$f'_{comp}(a) = [f(a+h)+E_+ - f(a-h) - E_-]/(2h) = [f(a+h)-f(a-h)]/(2h) + [E_+ - E_-]/(2h).$$

So we really have

$$f'(a) - f'_{comp}(a) = -h^2 f''(\xi)/6 - [E_+ - E_-]/(2h).$$

Thus the error consists of two parts, the discretization error (arising from approximating the derivative by a divided difference) and the roundoff error. As $h \to 0$, the discretization error $\to 0$. But if $E_+ - E_- \neq 0$, then $[E_+ - E_-]/(2h) \to \infty$. So, one must be careful not to take $h$ so small that the roundoff error becomes the dominant error in the computation.

7.3. **Numerical Differentiation using piecewise polynomials.** Just as piecewise polynomials offer a better way to approximate functions than using high degree polynomials, derivatives of piecewise polynomials offer an better alternative to approximate derivatives of functions.

Example: Using, $C^0$ piecewise linear functions, we could approximate $f'(x)$ on the subinterval $(x_{i-1}, x_i)$ by the derivative of the interpolant, i.e., by $[f(x_i) - f(x_{i-1})]/(x_i - x_{i-1})$. This approximation is defined everywhere except at the mesh points.

To obtain approximation to higher derivatives, we must start with a smoother piecewise polynomial. The space of $C^1$ piecewise cubics can be used to get approximations to $f'(x)$ everywhere and to $f''(x)$ everywhere except at the mesh points. The space of cubic splines will give approximations to $f''(x)$ everywhere and to $f^{(3)}(x)$ everywhere except at the mesh points.