Introduction to Numerical Differentiation & Richardson's Interpolation

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A sheet of corrugated roofing is constructed by pressing a flat sheet of aluminum into one whose cross section has the form of a sine wave.

A corrugated sheet 4 ft long is needed, the height of each wave is 1 in. from the center line, and each wave has a period of approximately 2π in.

The problem of finding the length of the initial flat sheet is one of determining the length of the curve given by $f(x) = \sin x$ from $x = 0$ in. and $x = 48$ in. From calculus we know that this length is

$$L = \int_0^{48} \sqrt{1 + [f'(x)]^2} dx = \int_0^{48} \sqrt{1 + \cos^2 x} dx,$$

so the problem reduces to evaluating this integral.

Although the sine function is one of the most common mathematical functions, the calculation of its length involves an elliptic integral of the second kind, which cannot be evaluated by ordinary methods.

One reason for using algebraic polynomials to approximate an arbitrary set of data is that, given any continuous function defined on a closed interval, a polynomial exists that is arbitrarily close to the function at every point in the interval.

Also, the derivatives and intervals of polynomials are easily obtained and evaluated. It should not be surprising, then, that most procedures for approximating integrals and derivatives use the polynomials that approximate the function.

The derivative of the function f at x_0 is

$$f'(x) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

This formula gives an obvious way to generate an approximation of $f'(x)$.

That is, we simply compute

$$\frac{f(x_0 + h) - f(x_0)}{h}$$

for small values of h.

To approximate $f'(x_0)$, suppose first that $x_0 \in (a, b)$, where $f \in C^2[a, b]$, and that $x_1 = x_0 + h$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a, b]$.

We construct the first Lagrange polynomial

$$P(x) = \frac{(x - x_0 - h)}{-h} f(x_0) + \frac{(x - x_0)}{h} f(x_0 + h)$$

for f determined by x_0 and x_1, with its error

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

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

Differentiating gives

$$f'(x) = \frac{f(x_0 + h) - f(x_0)}{h} f(x_0) + D_x \left[\frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x)) \right].$$

So

$$f'(x) = \frac{f(x_0+h)-f(x_0)}{h} f(x_0) + \frac{2(x-x_0)-h}{2} f''(\xi(x)) + \frac{(x-x_0)(x-x_0-h)}{2} D_x[f''(\xi(x))],$$

hence

$$f'(x) \approx \frac{f(x_0+h)-f(x_0)}{h}.$$

One difficulty with this formula is that we have no information about

$$D_x[f''(\xi(x))],$$

so the truncation error cannot be estimated.

When x is x_0, however, the coefficient of $D_x[f''(\xi(x))]$ is 0, and the formula simplifies to

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

For small values of h, the difference quotient

$$\frac{f(x_0+h)-f(x_0)}{h}$$

can be used to approximate $f'(x_0)$ with an error bounded by $\frac{M|h|}{2}$, where M is a bounded on $|f''(x)|$ for $x \in [a, b]$.

This formula is known as the **forward difference formula** if $h > 0$ and the **backward difference formula** if $h < 0$.

To obtain general derivative approximation formulas, suppose that $\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$. Then

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

for some $\xi(x)$ in I, where $L_k(x)$ denotes the kth Lagrange coefficient polynomial for f at $x_0, x_1, \ldots, x_n$.

Differentiating this expression gives

$$f'(x) = \sum_{k=0}^{n} f(x_k)L_k'(x) + D_x\left[\frac{(x-x_0)\cdots(x-x_k)}{(n+1)!}f^{(n+1)}(\xi(x))\right] + + \frac{(x-x_0)\cdots(x-x_k)}{(n+1)!}D_x\left[f^{(n+1)}(\xi(x))\right].$$

We again have a problem estimating the truncation error unless x is one of the numbers x_j.

In this case, the term multiplying $D_x\left[f^{(n+1)}(\xi(x))\right]$ is 0, and the formula becomes

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L_k'(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\prod_{\substack{k=0\\k\neq j}}^{n}(x_j - x_k)$$

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

In general, using more evaluation points in the above equation produces greater accuracy.

We first derive some useful three-point formulas and consider aspects of their errors. Hence

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

for each $j = 0, 1, 2$, where the notation ξ_j indicates that this point depends on x_j.

The three formulas the above equation become especially useful if the nodes are equally spaced, that is, when

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h, \text{ for some } h \neq 0.$$

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, these formulas can also be expressed as

$$
\begin{aligned}
f'(x_0) &= \frac{1}{h}\left[\frac{-3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0),\\
f'(x_0+h) &= \frac{1}{h}\left[\frac{-1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{6}f^{(3)}(\xi_1),
\end{aligned}
$$

and

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

As a matter of convenience, the variable substitution x_0 for $x_0 + h$ is used in the middle equation to change this formula to an approximation fof $f'(x_0)$.

A similar change, x_0 for $x_0 + 2h$, is used in the last equation. This gives three formulas for approximating $f'(x_0)$

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

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

and

$$f'(x_0) = \frac{1}{2h}\Big[f(x_0-2h) - 4f(x_0+h) + 3f(x_0)\Big] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

Finally, note that since the last of these equations can be obtained from the first by simply replacaing h with $-h$, there are actually only two formulas

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

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

$$f'(x_0) = \frac{1}{2h}\Big[f(x_0+h) - f(x_0-h)\Big] + \frac{h^2}{6}f^{(3)}(\xi_1), \quad (2)$$

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

Although the erros in both equations (1) and (2) are $O(h^2)$, the error in equation (2) is approximately half the error in (1). This is because equation (2) uses data on both sides of x_0 and equation (1) uses data on only one side.

Note also that f needs to be evaluated at only two points in equation (2), whereas in equation (1) three evaluations are needed.

The approximation in equation (1) is useful near the ends of an interval, since information about f outside the interval may not be available.

The methods presented in equations (1) and (2) are called **three-point formulas**.

Similarly, there are **five-point formulas** that involve evaluating the function at two more points, whose error term is $O(h^4)$. One is

$$f'(x_0) = \frac{1}{22h}\left[f(x_0 - 2h) - 8f(x_0 - h) - 8f(x_0 + 2h)\right] + \frac{h^4}{30}f^{(5)}(\xi),$$

where ξ lies between $x_0 + 2h$ and $x_0 + 2h$.

The other five point formula is useful for end point approximations. It is

$$f'(x_0) = \frac{1}{22h}\Big[-25f(x_0) - 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h) + \frac{h^4}{5}f^{(5)}(\xi),$$

where ξ lies between x_0 and $x_0 + 4h$.

Left end point approximations are found using this formula with $h > 0$ and **right end point approximations** with $h < 0$.

Methods can also be derived to find approximations to higher derivatives of a function using only tabulated values of the function at various points. The derivation is algebraically tedious, however, so only a representative procedure will be presented.

Expand a funtion f in a third Taylor polynomial about a point x_0 and evaluate $x_0 + h$ and $x_0 - h$. Then

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

and

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

where $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

If we add these equations, the terms involving $f'(x_0)$ and $f''(x_0)$ cancel and so,

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

Solving this equation for $f''(x_0)$ gives

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

Suppose $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$.

Since $\frac{1}{h^2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the intermediate value theorem implies that a number ξ exists between ξ and ξ_{-1}, and hence in $(x_0 - h, x_0 + h)$, with

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

Thus

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

for some ξ, where $x_0 - h < \xi < x_0 + h$.

Since $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$ it is also bounded, so the approximation is $O(h^2)$.

Richardson's Extrapolation

Richardson's extrapolation is used to generate high-accuracy results while using low-order formulas.

Extrapolation can be applied whenever it is known that an approximation technique has an error term with a predictable form, one that depends on a parameter, usually the step size h.

Suppose that for each number $h \neq 0$ we have a formula $N(h)$ that approximates an unknown value M and that the truncation error involved with the approximation has the form

$$M - N(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots ,$$

for some collection of unknown constants $K_1, K_2, K_3, \ldots$.

Since the truncation error is $O(h)$, we would expect, for example, that

$$M - N(0.1) \approx 0.1\ K_1, \qquad M - N(0.01) \approx 0.01\ K_1,$$

and in general, $M - N(h) = K_1\ h$, unless there was a large variation in magnitude among the constants $K_1, K_2, K_3, \ldots$.

The object of extrapolation is to find an easy way to consider the rather inaccurate $O(h)$ approximations in an appropriate way to produce formulas with a higher-order truncation error. Suppose, for example, we can combine the $N(h)$ formulas to produce an $O(h^2)$ approximation formula, $\tilde{N}(h)$, for M with

$$M - \tilde{N}(h) = \tilde{K}_1 h + \tilde{K}_2 h^2 + \tilde{K}_3 h^3 + \cdots,$$

for some, again unknown, collection of constants $\tilde{K}_1, \tilde{K}_2, \tilde{K}_3, \ldots$. Then we have

$$M - \tilde{N}(0.1) \approx 0.01\ \tilde{K}_2, \qquad M - \tilde{N}(0.01) \approx 0.0001\ \tilde{K}_2,$$

and so on.

If the constants K_1 and $\tilde{K}_2$ are roughly the same magnitude, then the $\tilde{N}(h)$ approximations.

The extrapolation continues by combining the $\tilde{N}(h)$ approximations in a manner that produces formulas with $O(h^3)$ truncation error, and so on.

To see specifically how we can generate these higher-order formulas, let us consider the formula for approximating M of the form

$$M = N(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots .$$

Since the formula is assumed to hold for all positive h, consider the result when we replace the parameter h by half its value. Then we have the formula

$$M = N\left(\frac{h}{2}\right) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots .$$

Eliminating the term K_1, we get

$$M = \left[2N\left(\frac{h}{2}\right) - N(h)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots .$$

To facilitate the discussion, we define $N_1(h) \equiv N(h)$ and

$$N_2(h) = \left[2N_1\left(\frac{h}{2}\right) - N_1(h)\right] = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right].$$

Then we have the $O(h^2)$ approximation formula for M:

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{3}h^3 - \cdots .$$

If we now replace h by $h/2$ in this formula, we have

$$M = N_2\left(\frac{h}{2}\right) - \frac{K_2}{8}h^2 - \frac{3K_3}{32}h^3 - \cdots .$$

Eliminating h^2 terms, we get

$$3M = 4N_2\left(\frac{h}{2}\right) - N_2(h) + \frac{3K_3}{8}h^3 + \cdots ,$$

and dividing by 3 gives an $O(h^3)$ formula for approximating M:

$$M = \left[N_2\left(\frac{h}{2}\right) + \frac{N_2(h/2) - N_2(h)}{3}\right] + \frac{K_3}{8}h^3 + \cdots .$$

By defining

$$N_3(h) \equiv N_2\left(\frac{h}{2}\right) + \frac{N_2(h/2) - N_2(h)}{3},$$

we have the $O(h^3)$ formula :

$$M = N_3(h) + \frac{K_3}{8}h^3 + \cdots .$$

The process is continued by construction an $O(h^4)$ approximation

$$N_4(h) = N_3\left(\frac{h}{2}\right) + \frac{N_3(h/2) - N_3(h)}{7},$$

an $O(h^5)$ approximation

$$N_5(h) = N_4\left(\frac{h}{2}\right) + \frac{N_4(h/2) - N_4(h)}{15},$$

and so on.

In general, if M can be written in the form

$$M = N5(h) + \sum_{j=1}^{m-1} K_j h^j + O(h^m),$$

then for each $j = 2, 3, \ldots, m$, we have an $O(h^j$ approximation of the form

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}.$$

These approximations are generated by rows in the order indicated by the numbered entries in the following table. This is done to take best advantage of the highest-order formulas.

$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^4)$
1: $N_1(h) \equiv N(h)$			
2: $N_1\left(\frac{h}{2}\right) \equiv N\left(\frac{h}{2}\right)$	**3:** $N_2(h)$		
4: $N_1\left(\frac{h}{4}\right) \equiv N\left(\frac{h}{4}\right)$	**5:** $N_2\left(\frac{h}{2}\right)$	**6:** $N_3(h)$	
7: $N_1\left(\frac{h}{8}\right) \equiv N\left(\frac{h}{8}\right)$	**8:** $N_2\left(\frac{h}{4}\right)$	**9:** $N_3\left(\frac{h}{2}\right)$	**10:** $N_4(h)$

Extrapolation can be applied whenever the truncation error for a formula has the form

$$\sum_{j=1}^{m-1} K_j h^{\alpha_j} + O(h^{\alpha_m}),$$

for a collection of constants K_j and when $\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m$.

References

- Richard L. Burden and J. Douglas Faires, "*Numerical Analysis – Theory ad Applications*", Cengage Learning, New Delhi, 2005.
- Kendall E. Atkinson, "*An Introduction to Numerical Analysis*", John Wiley & Sons, Delhi, 1989.