Numerical Differentiation

April 30, 2007

The derivative of a function f at the point x_0 is computed from

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

This formula suggests that the expression

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

for small values of h serves as an approximation of $f'(x_0)$:

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h}. \tag{1}$$

The approximation quality of this formula, however, is quite low due to round off errors. In this section we will learn how to obtain more accurate approximations of the derivative.

1 Differentiation and the Lagrange Polynomials

Recall that if $f \in C^{n+1}[a,b]$ and $x_0 < x_1 < \ldots < x_n \in [a,b]$, then we can write

$$f(x) = P_n(x) + \prod_{k=0}^{n} \frac{(x-x_k)}{(n+1)!} f^{(n+1)}(\xi(x)), \tag{2}$$

where $P_n(x)$ is the Lagrange polynomial interpolating f at the nodes $x_0, x_1, \ldots, x_n$:

$$P_n(x) = \sum_{k=0}^{n} f(x_k) L_{k,n}(x)$$

and $L_{k,n}(x)$ are the basic Lagrange polynomials

$$L_{k,n}(x) = \prod_{j\neq k}^{n} \frac{(x-x_k)}{(x_k-x_j)}$$

The approximation (1) can be obtained from the representation (2) as follows.

Put $n = 1, x_0 < x_1 \in [a, b]$ and $h = x_1 - x_0$. Then, from (2) we have

$$\begin{aligned} f(x) &= f(x_0)\frac{(x-x_1)}{(x_0-x_1)} + f(x_1)\frac{(x-x_0)}{(x_1-x_0)} + \frac{(x-x_0)(x-x_1)}{2}f''(\xi(x)) \\ &= f(x_0)\frac{(x-x_0-h)}{-h} + f(x_0+h)\frac{(x-x_0)}{h} + \frac{(x-x_0)(x-x_0-h)}{2}f''(\xi(x)) \\ &= f(x_0) + \frac{f(x_0+h)-f(x_0)}{h}(x-x_0) + \frac{(x-x_0)(x-x_0-h)}{2}f''(\xi(x)). \end{aligned}$$

Differentiating both sides with respect to x, we get

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

In particular, at $x = x_0$,

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2}f''(\xi_0),$$

where $\xi_0 \in (x_0, x_1)$.

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

with an approximation error of the order $O(h)$. In the following subsection we generalize this procedure.

1.1 General Approximation Formulas

Differentiation equation (2) with respect to x gives

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

In particular, for $x = x_r$ we have

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

This formula is called the $(n+1)$-point formula for approximating $f'(x_r)$. Of particular interest are the 3 and 5-point formulas.

1.2 3-point and 5-point formulas

From now on we will assume that the nodes are equally spaced with space step h, so that $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$ and so on. To obtain the 3-point formula, we put $n = 2$ in

(3) and simplify. We have

$$L_{0,2}(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{1}{2h^2}(x-x_1)(x-x_2), \qquad L'_{0,2}(x) = \frac{2x-x_1-x_2}{2h^2},$$
$$L_{1,2}(x) = \frac{(x-x_2)(x-x_0)}{(x_1-x_2)(x_1-x_0)} = -\frac{1}{h^2}(x-x_0)(x-x_2), \qquad L'_{1,2}(x) = -\frac{2x-x_0-x_2}{h^2},$$
$$L_{2,2}(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{1}{2h^2}(x-x_0)(x-x_1), \qquad L'_{2,2}(x) = \frac{2x-x_0-x_1}{2h^2}.$$

Hence,

$$\begin{aligned} f'(x_0) &= -\frac{3}{2h}f(x_0) + \frac{2}{h}f(x_1) - \frac{1}{2h}f(x_2) + \frac{h^2}{3}f^{(3)}(\xi_0) \\ &= \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0), \end{aligned}$$

and similarly,

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

If, in each one of the latter two formulas we replace x_0+h, and x_0+2h by x_0 they become

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

Next we observe that the third of these formulas is obtained from the first one by replacing h by $-h$, so that we really have two formulas

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

$$f'(x_0) \approx \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right]. \tag{5}$$

Formula (4) is useful at the end-points of the interval $[a,b]$ while formula (5) is useful at interior points of the interval. We should also notice that, although both formulas are $O(h^2)$, the error in using formula (5) is about half as much as the error in using formula (4). This is due to the fact that formula (5) uses information on both sides of x_0, while formula (4) uses information only on one side of x_0. Furthermore, (5) uses only two function evaluations while (4) uses three function evaluations.

5-point formulas are obtained in a similar fashion and we have

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30}f^{(5)}(\xi), \quad (6)$$

where $\xi \in (x_0-2h, x_0+2h)$ and

$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] + \frac{h^4}{5}f^{(5)}(\eta),$$

where $\eta \in (x_0, x_0+4h)$. Again, the last formula is used (with $h > 0$) at the left end-point and (with $h < 0$) at the right end-point.

Example The following table gives the values of the function $f(x) = xe^x$.

x	$y = xe^x$
1.8	10.88936544
1.9	12.70319944
2	14.7781122
2.1	17.14895682
2.2	19.8550297

Approximate $f'(2)$ and $f'(1.8)$ using two point, 3point and 5-point formulas.

Using the two point formula, we have

$$f'(2) \approx \frac{f(2.1) - f(2)}{0.1} = 23.70844619.$$

with the 3-point formula, we get

$$f'(2) \approx \frac{1}{0.2}\left[f(1.9) + f(2.1)\right] = 22.22878688$$

and

$$f'(2) \approx \frac{1}{1.2}\left[f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)\right] = 22.16699562$$

Since $f'(x) = (x+1)e^x$, $f'(2) = 3e^2 = 22.1671683$. The absolute error of using the two point formula is $1.541\,3$, of using the three point formula is $6.161\,9 \times 10^{-2}$ and of using the five point formula is $1.726\,8 \times 10^{-4}$. Obviously, the two point formula is very inaccurate and in order to obtain higher accuracy using this formula one has to take much smaller h which will result in a higher round off error.

For the point 1.8, we have

$$\begin{aligned} f'(1.8) &\approx \frac{f(1.8) - f(1.9)}{0.1} = 18.13834004 \text{ (using the two point formula)} \\ &\approx \frac{1}{.1}\left[-\frac{3}{2}f(1.8) + 2f(1.9) - \frac{1}{2}f(2)\right] \\ &= 16.83294628 \text{ (using the three point formula)} \\ &\approx \frac{1}{1.2}\left[-25f(1.8) + 48f(1.9) - 36f(2) + 16f(2.1) - 3f(2.2)\right] \\ &= 16.93801507 \text{ (using the five point formula)} \end{aligned}$$

The errors are 1.1993, 1.0607×10^{-1} and 9.9783×10^{-4}, respectively.

1.3 Richardson's Extrapolation

Richardson's extrapolation is used to obtain high accuracy results while using low-order formulas. For ease of reference, we let $f_k = f(x_k) = f(x_0 + kh)$. We also let

$$D_0(h) = \frac{f_1 - f_{-1}}{2h}.$$

Then, using formula (3) we may write

$$f'(x_0) \approx D_0(h) + Ch^2.$$

Hence,

$$f'(x_0) \approx D_0(2h) + 4Ch^2$$

Multiplying the first equation by 4 and subtracting the second equation from it we get

$$\begin{aligned} 3f'(x_0) &\approx 4D_0(h) - D_0(2h) \\ &= 4\frac{f_1 - f_{-1}}{2h} - \frac{f_2 - f_{-2}}{4h} \\ &= \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{4h}. \end{aligned}$$

Solving for $f'(x_0)$ we get

$$f'(x_0) \approx \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}.$$

Observe that this expression is the same as (6) therefore, the approximation here is $O(h^4)$. In summary then, we can use the $O(h^2)$ expression $D_0(h)$ to obtain $O(h^4)$ approximation of $f'(x_0)$ by

$$f'(x_0) \approx \frac{4D_0(h) - D_0(2h)}{3}.$$

Example Let $f(x) = xe^x$, $x_0 = 2$, $h = 0.1$ Then

$$\begin{aligned} D_0(h) &= \frac{f(2.1) - f(1.9)}{.2} = 22.22878688, \\ D_0(2h) &= \frac{f(2.2) - f(1.8)}{.4} = 22.41416066, \\ f'(x_0) &\approx \frac{4D_0(h) - D_0(2h)}{3} = \frac{4(22.22878688) - 22.41416066}{3} \\ &= 22.16699562. \end{aligned}$$

The exact value of $f'(x) = 22.1671683$; the absolute error is 0.000172675.

The above process to obtain $O(h^4)$ approximation can be repeated to obtain a higher order formula as follows. Let

$$D_1(h) = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}.$$

Then

$$f'(x_0) \approx D_1(h) + Ch^4.$$

Then

$$f'(x_0) \approx D_1(2h) + 16Ch^4$$

and

$$15f'(x_0) \approx 16D_1(h) - D_1(2h),$$

so that

$$f'(x_0) \approx \frac{16D_1(h) - D_1(2h)}{15}.$$

The error in this case is $O(h^6)$. The general pattern is:

> If $f'(x_0) \approx D_{k-1}(h)$ with error $O\left(h^{2k}\right)$, then
>
> $$f'(x_0) \approx \frac{4^k D_{k-1}(h) - D_{k-1}(2h)}{4^k - 1}$$
>
> with error $O\left(h^{2k+2}\right)$.

2 Higher Order Derivatives

In the last section we discussed how to obtain approximations of the first derivative of a function f at a point x_0 with high levels of accuracy. The same approach can be used to obtain approximations of higher derivatives of f. The derivations are tedious, though. The following tables list some central difference and endpoint difference formulas for higher derivatives.

Central difference formulas of order $O(h^2)$:

$$\begin{aligned} f'(x_0) &\approx \frac{f_1 - f_{-1}}{2h} \\ f''(x_0) &\approx \frac{f_1 - 2f_0 - f_{-1}}{h^2} \\ f^{(3)}(x_0) &\approx \frac{f_2 - 2f_1 + 2f_{-1} - f_{-2}}{2h^3} \\ f^{(4)}(x_0) &\approx \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4}. \end{aligned}$$

Central difference formulas of order $O\left(h^4\right)$:

$$
\begin{aligned}
f'\left(x_0\right) &\approx \frac{-f_2+8f_1-8f_{-1}+f_{-2}}{12h}\\
f''\left(x_0\right) &\approx \frac{-f_2+16f_1-30f_0+16f_{-1}-f_{-2}}{12h^2}\\
f^{(3)}\left(x_0\right) &\approx \frac{-f_3+8f_2-13f_1+13f_{-1}-8f_{-2}+f_{-3}}{8h^3}\\
f^{(4)}\left(x_0\right) &\approx \frac{-f_3+12f_2-39f_1+56f_0-39f_{-1}+12f_{-2}-f_{-3}}{6h^4}.
\end{aligned}
$$

Left end-point differences (forward differences) of order $O\left(h^2\right)$:

$$
\begin{aligned}
f'\left(x_0\right) &\approx \frac{-3f_0+4f_1-f_2}{2h}\\
f''\left(x_0\right) &\approx \frac{2f_0-5f_1+4f_2-f_3}{h^2}\\
f^{(3)}\left(x_0\right) &\approx \frac{-5f_0+18f_1-24f_2+14f_3-3f_4}{2h^3}\\
f^{(4)}\left(x_0\right) &\approx \frac{3f_0-14f_1+26f_2-24f_3+11f_4-2f_5}{h^4}.
\end{aligned}
$$

For right end-points, replace h by $-h$.