Numerical differentiation

We all know what is differentiation:

$$\frac{d}{dx}f(x) = f'(x)$$

The function $f(x)$ may ba a function known analytically, or a set of discrete data. For the functions known explicitly the differentiation is straightforward while differentiation of discrete data requires an approximate numerical procedure.
Most common numerical procedures are based on fitting approximating functions to a set of discrete data with subsequent differentiation of the approximating function; for example

$$\frac{d}{dx}f(x) = \frac{d}{dx}P_n(x)$$

where $P_n(x)$ is an approximating polynomial.

Even though the approximating polynomial $P_n(x)$ passes through the discrete data points exactly, the derivative of the polynomial $P_n'(x)$ may not be a very accurate approximation of the derivative of the exact function $f(x)$, even at the known data points.

Numerical differentiation

In general, numerical differentiation is an inaccurate process. Numerical differentiation procedures:

1. Differentiation of direct fit polynomials.
2. Differentiation of Lagrange polynomials.
3. Differentiation of divided difference polynomials
4. Differentiation of Newton forward-difference or Newton backward-difference polynomials on equally spaced x_i.
5. Differentiation of based on Taylor series. This approach is very useful in numerical solutions of differential equations.

Three straightforward numerical differentiation procedures that can be used for both unequally and equally spaced data are:

1. Direct fit polynomials.
2. Lagrange polynomials.
3. Divided difference polynomials

Accuracy of polynomial approximation

Theorem.
Suppose that $x_0, x_1, ..., x_N$ are N +1 distinct numbers in the interval [a, b]. and $[x_j, f(x_j]$ is a set of data. There exists a unique polynomial $P_N(x)$ of degree at most N with the property that

$$f(x_j) = P_N(x_j) \quad \text{for} \;\; j = 0, 1, ..., N.$$

The Newton form of this polynomial is

$$P_N(x) = a_0 + a_1(x - x_0) + ... + a_N(x - x_0)(x - x_1)(x - x_{N-1}),$$

where $a_k = f[x_0, x_1, ..., x_k]$ for k = 0, 1, . . . , N are divided differences

Corollary (Newton Approximation).
Assume that $P_N(x)$ is the Newton polynomial given in the above theorem and it is used to approximate the function f(x):

$$f(x) = P_N(x) + E_N(x).$$

If f is differentiable $N + 1$ times at $[a, b]$, then for each $x \in [a, b]$ there exists a number c = c(x) in (a, b), so that the error term has the form

$$E_N(x) = (x - x_0)(x - x_1)....(x - x_N)\frac{f^{(N+1)}(c)}{(N+1)!}.$$

Not that the error term $E_N(x)$ is the same as the one for Lagrange interpolation.

Direct fit polynomials

The direct fit polynomials are

$$P_n(x) \;=\; a_0 + a_1 x + a_2 x^2 + ... + a_n x^n$$

For $N = n + 1$ points the set $\{x_i, f(x_i)\}$ determines the exact nth-degree polynomial with best fit to the data points. After that, $f'(x)$ is simply

$$\begin{aligned} f'(x) \;&\simeq\; P'_n(x) \;=\; a_1 + 2a_2 x + 3a_3 x^2 + ... + n a_n x^{n-1} \\ f''(x) \;&\simeq\; P''_n(x) \;=\; 2a_2 + 6a_3 x^2 + ... + n(n-1) a_n x^{n-2} \end{aligned}$$

etc.

Lagrange polynomials

Example: second-degree Lagrange polynomial

$$
\begin{aligned}
P_2(x) &= \frac{(x-b)(x-c)}{(a-b)(a-c)}f(a) + \frac{(x-a)(x-c)}{(b-a)(b-c)}f(b) + \frac{(x-a)(x-b)}{(c-a)(c-b)}f(c) \\
f'(x) \simeq P_2'(x) &= \frac{2x-b-c}{(a-b)(a-c)}f(a) + \frac{2x-a-c}{(b-a)(b-c)}f(a) + \frac{2x-a-b}{(c-a)(c-b)}f(c) \\
f''(x) \simeq P_2''(x) &= \frac{2f(a)}{(a-b)(a-c)} + \frac{f(b)}{(b-a)(b-c)} + \frac{2f(c)}{(c-a)(c-b)}
\end{aligned}
$$

Divided difference polynomials

$$
\begin{aligned}
P_n(x) \;&=\; f_i^{(0)} + (x - x_i)f_i^{(1)} \\
&\quad + (x - x_i)(x - x_{i+1})f_i^{(2)} + (x - x_i)(x - x_{i+1})(x - x_{i+2})f_i^{(3)} + ..., \\
f'(x) \;\simeq\; P_n'(x) \;&=\; f_i^{(1)} + (2x - x_i - x_{i+1})f_i^{(2)} \\
&\quad + (3x^2 - 2xx_i - 2xx_{i+1} - 2xx_{i+2} + (x_i x_{i+1} + x_i x_{i+2} + x_{i+1}x_{i+2})f_i^{(3)} + ..., \\
f''(x) \;\simeq\; P_n''(x) \;&=\; 2f_i^{(2)} + (6x - 2x_i - 2x_{i+1} - 2x_{i+2})f_i^{(3)} + ...
\end{aligned}
$$

Equally spaced data: Newton polynomials

Newton forward-difference polynomials.

$$P_n(x) \equiv f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{6}\Delta^3 f_0 + \ldots$$

where $h = x_1 - x_0, \quad x = x_0 + sh,$
$\Delta^{(n)} f_0 = f_n - nf_{n-1} + \frac{(n(n-1)}{2} f_{n-2} + \ldots + (-1)^n f_0.$
We get

$$f'(x) \simeq P_n'(x) = \frac{dP_n(s)}{ds}\frac{ds}{dx} = \frac{1}{h}\frac{dP_n(s)}{ds}$$
$$P_n'(x) = \frac{1}{h}\left[\Delta f_0 + \frac{2s-1}{2}\Delta^2 f_0 + \frac{3s^2-6s+2}{6}\Delta^3 f_0 + \ldots\right]$$

In the second order

$$f''(x) \simeq \frac{d}{dx}P_n'(x) = \frac{1}{h}\frac{d^2 P_n(s)}{ds^2}$$
$$P_n''(x) = \frac{1}{h^2}\left[\Delta^2 f_0 + (s-1)\Delta^3 f_0 + \ldots\right]$$

As n increases, $\Delta^n f$ becomes less and less accurate.
In practical applications we usually need to know derivatives at the point x_0 $(s = 0)$, then

$$P_n'(x_0) = \frac{1}{h}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \frac{1}{4}\Delta^4 f_0 + \ldots\right]$$
$$P_n''(x_0) = \frac{1}{h^2}\left[\Delta^2 f_0 - \Delta^3 f_0 + \ldots\right]$$

Differentiation of Newton polynomials

Errors: differentiate the error term in divided differences.
For $s = 0$

$$\frac{d}{dx}[\text{error}(x_0)] \;=\; \frac{d}{dx}[E_n(x_0)] \;=\; \frac{1}{(n+1)!}h^n f^{(n+1)}(b), \qquad x_0 \le b \le x_n$$

Newton backward-difference polynomials.

$$\begin{aligned}
P_n(x) \;&=\; f_0 + s\nabla f_0 + \frac{s(s+1)}{2!}\nabla^2 f_0 + \frac{s(s+1)(s+2)}{3!}\nabla^3 f_0 + ... \\
P_n'(x) \;&=\; \frac{1}{h}[\nabla f_0 + \frac{2s+1}{2}\nabla^2 f_0 + \frac{3s^2+6s+2}{6}\nabla^3 f_0 + ...] \\
P_n''(x) \;&=\; \frac{1}{h^2}[\nabla^2 f_0 + (s+1)\nabla^3 f_0 + ...]
\end{aligned}$$

As n increases $\nabla^n f$ becomes less accurate.

$$\text{At } \; x = x_0 \qquad P_n'(x) \;=\; \frac{1}{h}[\nabla f_0 + \frac{1}{2}\nabla^2 f_0 + \frac{1}{3}\nabla^3 f_0 + ...],$$

$$P_n''(x) \;=\; \frac{1}{h^2}[\nabla^2 f_0 + \nabla^3 f_0 + ...]$$

Centered-difference formulas.

Example for $x = x_{-1}$, $s = -1.0$

$$\begin{aligned} P_n'(x_{-1}) &= \frac{1}{h}\left[\nabla f_0 - \frac{1}{2}\nabla^2 f_0 - \frac{1}{6}\nabla^3 f_0 + ...\right], \\ P_n''(x_{-1}) &= \frac{1}{h^2}\left[\nabla^2 f_0 - \frac{1}{12}\nabla^4 f_0 + ...\right] \end{aligned}$$

Centered-difference formulas.

There is a way to have better accuracy for $n \geq 2$ terms: centered-difference formulas.

$$\begin{aligned} P_n'(x_0) &= \frac{1}{h}\left[\delta f_0 + \frac{1}{2}\delta^2 f_0 - \frac{1}{6}\delta^3 f_0 + ...\right], \\ P_n''(x_0) &= \frac{1}{h^2}\left[\delta^2 f_0 + \frac{1}{12}\delta^3 f_0 + ...\right] \end{aligned}$$

Examples.

Divided differences are defined through function values. For specific order n it is straightforward to express divided differences in terms of function values. Below we present some results for the first and second orders.

One-sided forward difference

First-order derivative

$$P_1'(x_0) = \frac{f_1 - f_0}{h} + O(h)$$
$$P_2'(x) = \frac{-3f_0 + 4f_1 - f_2}{2h} + O(h)$$

Second-order derivative

$$P_2''(x_0) = \frac{f_2 - 2f_1 + f_0}{h^2} + O(h)$$
$$P_3''(x_0) = \frac{2_0 - 5f_1 + 4f_2 - f_3}{h^2} + O(h^2)$$

Centered-difference formulas

$$P_2'(x_1) = \frac{f_2 - f_0}{2h} + O(h^2)$$
$$P_2''(x_1) = \frac{f_0 - 2f_1 + f_2}{h^2} + O(h^2)$$

Analytic difference formulas at any order could be derived in a similar way.

Taylor series.

Taylor series enables us a to derive finite difference approximations for total and partial derivatives in differential equations.

$$f(x) \;=\; f_0 + \Delta x\, f_0' + \frac{\Delta x^2}{2} f_0'' + \frac{\Delta x^3}{6} f_0''' + ... + \frac{\Delta x^n}{n!} f_0^{(n)} + ...$$

where $f_0 \equiv f(x_0), f_0' \equiv f'(x_0), f_0'' \equiv f''(x_0)$ etc.

Taylor series for one variable:

$$f(t) \;=\; f(t_0) + \Delta t\, f'(t_0) + \frac{\Delta t^2}{2} f''(t_0) + ... + \frac{\Delta t^n}{n!} f^{(n)}(x_0) + ...$$

Taylor series for two variables:

$$\begin{aligned} f(x,t) \;=\; & f(x_0,t_0) + \Delta x\, f_x'(x_0,t_0) + \Delta t\, f_t'(x_0,t_0) \\ & + \frac{1}{2}\left[\Delta x^2 f_{xx}''(x_0,t_0) + 2\Delta x \Delta t\, f_{xt}''(x_0,t_0) + f_{tt}'' \Delta t^2 (x_0,t_0)\right] + ... \end{aligned}$$

The Taylor series for $f(x)$ (or $f(x,t)$) can be used to obtain difference formulas for f' (or f_x, f_t etc).

Derivatives using Taylor series.

Let us choose i as a base point for Taylor series

$$
\begin{aligned}
f_{i+1} &= f_i + \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' + \frac{\Delta x^3}{3!} f_i''' + \frac{\Delta x^4}{4!} f_i'''' + \ldots \\
f_{i-1} &= f_i - \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' - \frac{\Delta x^3}{3!} f_i''' + \frac{\Delta x^4}{4!} f_i'''' + \ldots\ldots
\end{aligned}
$$

$\Rightarrow$

$$
f_{i+1} - f_{i-1} = 2\Delta x f_i' + \frac{\Delta x^3}{3} f_i''' + \ldots, \qquad f_{i+1} + f_{i-1} = 2f_i + f_i'' \Delta x^2 + \frac{1}{12} \Delta x^4 f_i''''
$$

We can solve for f_i' and f_i''

$$
\begin{aligned}
f_i' &= \frac{f_{i+1} - f_{i-1}}{2\Delta x} - \frac{\Delta x^2}{6} f'''(b), & x_{i-1} \le b \le x_{i+1} \\
f_i'' &= \frac{f_{i+1} - 2f_i + f_{i-1}}{2\Delta x} - \frac{\Delta x^2}{12} f''''(b), & x_{i-1} \le b \le x_{i+1}
\end{aligned}
$$

Without the remainder terms the results are identical to those obtained from Newton divided-difference polynomial:

$$
P_2'(x_1) = \frac{f_2 - f_0}{2h} + O(h^2), \qquad P_2''(x_1) = \frac{f_0 - 2f_1 + f_2}{h^2} + O(h^2)
$$

Difference formulas at an arbitrary order can be obtained by combinations of Taylor series for $f(x)$ at various grid points. (Higher order difference formulas need more points)

General method for deriving difference formulas by Taylor series.

1. Choose n of the derivative $f^{(n)}$ for which the difference formula should be derived.
2. Choose the order r of the remainder in Δx^r.
3. Specify the type of difference formula (centered, forward, backward, non-symmetrical).
4. Determine the number of required grid points ($\simeq n + r - 1$).
5. Write the Taylor series of order $(n + r)$ at the $(n + r - 1)$ points.
6. Combine the Taylor series to eliminate the unwanted derivatives and solve for the necessary derivative.

Example

Third-order, non-symmetrical, backwards-biased difference formula for $f(x)$.

Let us take $n = 1$ and $r = 4$ so that we need $n + r - 1 = 4$ points (including base point). For a backward-difference we can choose points $i-2, i-1, i, i+1$ so Taylor series for these points have the form

$$
\begin{aligned}
f_{i+1} &= f_i + \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' + \frac{\Delta x^3}{6} f_i''' + \frac{\Delta x^4}{24} f_i'''' + \ldots \\
f_{i-1} &= f_i - \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' - \frac{\Delta x^3}{6} f_i''' + \frac{\Delta x^4}{24} f_i'''' + \ldots \\
f_{i-2} &= f_i - 2\Delta x f_i' + 2\Delta x^2 f_i'' - \frac{4\Delta x^3}{3} f_i''' + \frac{2\Delta x^4}{3} f_i'''' + \ldots
\end{aligned}
$$

Now we form the combinations

$$
\begin{aligned}
f_{i+1} - f_{i-1} &= 2\Delta x f_i' + \frac{\Delta x^3}{3} f_i''' + O(\Delta x^5) \\
4f_{i+1} - f_{i-2} &= 3f_i + 6\Delta x f_i' + 2\Delta x^3 f_i''' - \frac{\Delta x^4}{2} f_i'''' + \ldots \\
\Rightarrow f_i' &= \frac{f_{i-2} - 6f_{i-1} + 3f_i + 2f_{i+1}}{6\Delta x} - \frac{1}{2} f''''(b) \Delta x^3
\end{aligned}
$$

Error estimation and Richardson extrapolation

The error can be estimated by comparing the results for two different step sizes.
This error estimate can be used for error control and extrapolation improving the accuracy.

Consider a method which approaches an exact solution as

$$f_{\text{exact}} = f(h) + Ah^n + O(h^{n+m})$$

and for the step h/R

$$f_{\text{exact}} = f(h/R) + A\left(\frac{h}{R}\right)^n + O(h^{n+m})$$

Subtracting the second equation from the first one we get

$$0 = f(h) - f\left(\frac{h}{R}\right) + Ah^n - A\left(\frac{h}{R}\right)^n + O(h^{n+m})$$

and therefore

$$\text{Error}(h) = Ah^n = \frac{R^n}{R^n - 1}\big[f(h/R) - f(h)\big]$$

$$\text{Error}\big(h/R\big) = A(h/R)^n = \frac{1}{R^n - 1}\big[f(h/R) - f(h)\big]$$

$$\Rightarrow \text{ Extrapolated value } = f\left(\frac{h}{R}\right) + \frac{1}{R^n - 1}\big[f(h/R) - f(h)\big]$$

Example

We saw that Taylor Series of $f(x)$ about the point x_0 and evaluated at $x_0 + h$ and $x_0 - h$ leads to the central difference formula:

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f'''(x_0) - \frac{h^4}{120} f^{(5)}(x_0) + ...$$

This formula describes precisely how the error behaves. This information can be exploited to improve the quality of the numerical solution without ever knowing $f''', f^{(5)}$, ... (Recall that we have a $O(h^2)$ approximation)
Let us rewrite this in the following form:

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f'''(x_0) - \frac{h^4}{120} f^{(5)}(x_0) + ...$$

where

$$N(h) = \frac{f(x+h) - f(x-h)}{2h}$$

The key of the process is to now replace h by h/2 in this formula.

We find

$$f'(x_0) = N(h/2) - \frac{h^2}{24} f'''(x_0) - \frac{h^4}{1920} f^{(5)}(x_0) + .$$

Look closely at what we had from before:

$$f'(x) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f'''(x_0) - \frac{h^4}{120} f^{(5)}(x_0) + .$$

Careful substraction cancels a higher order term: take

$$4f'(x_0) = 4N(h/2) - 4\frac{h^2}{24} f'''(x_0) - 4\frac{h^4}{1920} f^{(5)}(x_0) + ...$$

add

$$-f'(x_0) = -N(h) + \frac{h^2}{6} f'''(x_0) + \frac{h^4}{120} f^{(5)}(x_0) + .$$

get

$$3f'(x_0) = 4N(h/2) - N(h) + \frac{h^4}{160} f^{(5)}(x_0) + ...$$

Thus

$$f'(x_0) \;=\; N(h/2) + \frac{N(h/2) - N(h)}{3} + \frac{h^4}{160} f^{(5)}(x_0)$$

is an $O(h^4)$ formula.

Notice what we have done. We took two $O(h^2)$ approximations and created a $O(h^4)$ approximation. We did require, however, that we have functional evaluations at h and h/2.
This approximation requires roughly twice as much work as the second order centered difference formula.
However, the truncation error now decreases much faster with h.