# 1 Problem

A function $f(x)$ is known at $x_i$ and the corresponding values are $f_i$ $(i = 1, \ldots, n)$. Find the finite difference formulae at $x_i$ to approximate the derivatives of $f(x)$ to the highest accuracy.

# 2 Answer

Let us first look at an interpolation problem: find a polynomial $P(x)$ of highest order $n-1$ such that $P(x_i) = f_i$. This problem can be solved by using Lagrange polynomials

$$P(x) = \sum_u f_u L_u(x) \quad L_i(x) = \prod_{\imath \neq i} \frac{x - x_\imath}{x_i - x_\imath}$$

in which $L_i(x)$ has a property that $L_i(x_j) = \delta_{ij}$. There is a nice introduction about Lagrange polynomial in `https://en.wikipedia.org/wiki/Lagrange_polynomial`. We know such $P(x)$ is unique since polynomial space up to a certain order has a finite dimension.

What is the degree of accuracy by approximating $f(x)$ using $P(x)$? To answer this question, we first define $r(x) = f(x) - P(x)$, we know $r(x_i) = 0$. Write $r(x)$ in a multiplicative form

$$r(x) = s(x) \prod_u (x - x_u)$$

where $s(x)$ is an unknown function. Define another auxiliary function

$$g(t) = r(t) - s(x) \prod_u (t - x_u) = f(t) - P(t) - s(x) \prod_u (t - x_u)$$

We have $g(x) = 0$. Therefore, $g(t)$ has $n+1$ zero points. Recursively apply Rolle's theorem, we know $g^{(n)}(t)$ has at least one zero point $\xi$, $g^{(n)}(\xi) = 0$.

$$\begin{aligned}
g^{(n)}(\xi) &= \left.\frac{\mathrm{d}^n}{\mathrm{d}t^n}\right|_{t=\xi} \left( f(t) - P(t) - s(x) \prod_u (t - x_i) \right) \\
&= f^{(n)}(\xi) - P^{(n)}(\xi) - s(x) \left.\frac{\mathrm{d}^n}{\mathrm{d}t^n}\right|_{t=\xi} \prod_u (t - x_i) \\
&= f^{(n)}(\xi) - s(x) n!
\end{aligned}$$

Solve for $s(x)$, we get

$$s(x) = \frac{f^{(n)}(\xi)}{n!}$$

Therefore

$$f(x) = P(x) + \frac{f^{(n)}(\xi)}{n!} \prod_u (x - x_u)$$

We call $P(x)$ approximates $f(x)$ to the $n-1$-th order. Recall the definition of order of accuracy in finite difference, we realize that if we use $P^{(m)}(x_i)$ to approximate $f^{(m)}(x_i)$ $(1 \leq m \leq n)$, this approximation has an accuracy to the order of $n-1$.

So the whole idea is to find a polynomial that is "close" enough to the unknown function, then calculate the derivatives of this polynomial and evaluate the derivatives of this polynomial at known points to approximate the true derivatives of the unknown function.

Take $n = 2$ to have a close look

$$L_1(x) = \frac{x - x_2}{x_1 - x_2} \quad L_2(x) = \frac{x - x_1}{x_2 - x_1}$$

Then

$$
\begin{aligned}
P(x) &= f_1 \frac{x - x_2}{x_1 - x_2} + f_2 \frac{x - x_1}{x_2 - x_1} \\
P'(x) &= f_1/(x_1 - x_2) + f_2/(x_2 - x_1) = \frac{f_2 - f_1}{x_2 - x_1}
\end{aligned}
$$

We come to the finite difference of first order using two points. Revisit the formula of finite difference

$$
f'(x_1) \approx \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{1}{x_1 - x_2} f(x_1) + \frac{1}{x_2 - x_1} f(x_2)
$$

The equivalence to the interpolation problem is clear.

As discussed above, calculating the finite difference from known pairs $(x_i, f_i)$ is equivalent to calculate the derivatives of the corresponding interpolation polynomial. To write down the explicit form of the first two orders of finite differences using $n$ points, we first calculate the first two order derivatives of Lagrange polynomial (eliminate common factors in the multiplication)

$$
\begin{aligned}
L_i'(x) &= L_i(x) \sum_{\imath \neq i} \frac{1}{x - x_\imath} \\
&= \prod_{\imath' \neq i} \frac{x - x_{\imath'}}{x_i - x_{\imath'}} \sum_{\imath \neq i} \frac{1}{x - x_\imath} \\
&= \sum_{\imath \neq i} \frac{1}{x - x_\imath} \prod_{\imath' \neq i} \frac{x - x_{\imath'}}{x_i - x_{\imath'}} \\
&= \sum_{\imath \neq i} \frac{1}{x - x_\imath} \frac{x - x_\imath}{x_i - x_\imath} \prod_{\imath' \neq i, \imath} \frac{x - x_{\imath'}}{x_i - x_{\imath'}} \\
&= \sum_{\imath \neq i} \frac{1}{x_i - x_\imath} \prod_{\imath' \neq i, \imath} \frac{x - x_{\imath'}}{x_i - x_{\imath'}}
\end{aligned}
$$

$$
\begin{aligned}
L_i''(x) &= L_i(x) \left[ \left( \sum_{\imath \neq i} \frac{1}{x - x_\imath} \right)^2 - \sum_{\imath \neq i} \frac{1}{(x - x_\imath)^2} \right] \\
&= L_i(x) \sum_{\substack{\imath_1, \imath_2 \neq i \\ \imath_1 \neq \imath_2}} \frac{1}{(x - x_{\imath_1})(x - x_{\imath_2})} \\
&= \prod_{\imath' \neq i} \frac{x - x_{\imath'}}{x_i - x_{\imath'}} \sum_{\substack{\imath_1, \imath_2 \neq i \\ \imath_1 \neq \imath_2}} \frac{1}{(x - x_{\imath_1})(x - x_{\imath_2})} \\
&= \sum_{\substack{\imath_1, \imath_2 \neq i \\ \imath_1 \neq \imath_2}} \frac{1}{(x - x_{\imath_1})(x - x_{\imath_2})} \prod_{\imath' \neq i} \frac{x - x_{\imath'}}{x_i - x_{\imath'}} \\
&= \sum_{\substack{\imath_1, \imath_2 \neq i \\ \imath_1 \neq \imath_2}} \frac{1}{(x - x_{\imath_1})(x - x_{\imath_2})} \frac{x - x_{\imath_1}}{x_i - x_{\imath_1}} \frac{x - x_{\imath_2}}{x_i - x_{\imath_2}} \prod_{\imath' \neq i, \imath_1, \imath_2} \frac{x - x_{\imath'}}{x_i - x_{\imath'}} \\
&= \sum_{\substack{\imath_1, \imath_2 \neq i \\ \imath_1 \neq \imath_2}} \frac{1}{(x_i - x_{\imath_2})(x_i - x_{\imath_2})} \prod_{\imath' \neq i, \imath_1, \imath_2} \frac{x - x_{\imath'}}{x_i - x_{\imath'}}
\end{aligned}
$$

Then $f'(x)$ and $f''(x)$ are approximated as

$$
f'(x) \approx \sum_u f_u \sum_{\imath \neq u} \frac{1}{x_u - x_\imath} \prod_{\imath' \neq u, \imath} \frac{x - x_{\imath'}}{x_u - x_{\imath'}}
$$

$$f''(x) \approx \sum_u f_u \sum_{\substack{\imath_1, \imath_2 \neq u \\ \imath_1 \neq \imath_2}} \frac{1}{(x_u - x_{\imath_2})(x_u - x_{\imath_2})} \prod_{\imath' \neq u, \imath_1, \imath_2} \frac{x - x_{\imath'}}{x_u - x_{\imath'}}$$

Therefore the first two orders of finite differences $f'(x_i)$ and $f''(x_i)$ are

$$f'(x_i) \approx \sum_u f_u \sum_{\imath \neq u} \frac{1}{x_u - x_\imath} \prod_{\imath' \neq u, \imath} \frac{x_i - x_{\imath'}}{x_u - x_{\imath'}}$$

$$f''(x_i) \approx \sum_u f_u \sum_{\substack{\imath_1, \imath_2 \neq u \\ \imath_1 \neq \imath_2}} \frac{1}{(x_u - x_{\imath_1})(x_u - x_{\imath_2})} \prod_{\imath' \neq u, \imath_1, \imath_2} \frac{x_i - x_{\imath'}}{x_u - x_{\imath'}}$$