

Basic Numerical Methods

by

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Numerical Differentiation

A numerical derivative can be derived using the following approach:

The Taylor Series for $f(x)$ about the point $x = a$ is given by equation (1)

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!} f''(a) + \dots + \frac{(x-a)^n}{(n-1)!} f^{(n)}(a) + R_n \quad (1)$$

If we quantize $f(x)$ by setting $x_n = nh$ for $n \equiv$ an integer and $h \equiv \Delta x$ then $f_n = f(x_n)$

(2)

We set $a = 0$ then

$$f_1 = f(h) = f(0) + f'(0)h + f''(0)\frac{h^2}{2!} + f'''(0)\frac{h^3}{3!} + O(h^4) \quad (3)$$

$$f_{-1} = f(-h) = f(0) - f'(0)h + f''(0)\frac{h^2}{2!} - f'''(0)\frac{h^3}{3!} + O(h^4) \quad (4)$$

Subtracting equation (4) from equation (3) gives

$$f_1 - f_{-1} = 2 \left(f'(0)h + f'''(0)\frac{h^3}{3!} + O(h^4) \right) \quad (5)$$

Equation (5) can be rewritten as

$$f'(0) = \frac{f_1 - f_{-1}}{2h} - f'''(0)\frac{h^2}{6} + O(h^4) \quad (6)$$

For a general quantized point x_n , equation (6) gives

$$f'(x_n) = \frac{f_{n+1} - f_{n-1}}{2h} - f'''(x_n)\frac{h^2}{6} + O(h^4) \text{ or}$$

$$f'(x_n) \cong \frac{f_{n+1} - f_{n-1}}{2h} \quad (7)$$

Equation (7) will work when $f'''(x_n) \cong 0$. If $f'''(x_n) = 0$, then $f(x)$ is implicitly modeled by a second order polynomial. Higher order derivatives can be derived in the same way.

Numerical Integration

We start with the Taylor series using equation (1) with $a = 0$, use equation (7) for $f'(x_n)$ and use equation (8) for $f''(x_n)$.

$$f''(x_n) \approx \frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} \quad (8)$$

$$\text{Then } f(x_n) \approx f_n + \frac{f_{n+1} - f_{n-1}}{2h} x_n + \frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} \frac{x_n^2}{2!} \quad (9)$$

$$\begin{aligned} \int_{-h}^{+h} f(x_n) dx &= \left[f_n x + \frac{f_{n+1} - f_{n-1}}{2h} \frac{x_n^2}{2} + \frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} \frac{x_n^3}{6} \right]_{-h}^h = \\ 2f_n + \frac{h}{3} [f_{n+1} - 2f_n + f_{n-1}] &= \frac{h}{3} [f_{n+1} + 6f_n - 2f_n + f_{n-1}] = \\ \frac{h}{3} [f_{n+1} + 4f_n + f_{n-1}] \end{aligned} \quad (10)$$

which is Simpson's Rule. Higher order integration methods can be derived in a similar way. For a general discussion on this approach for deriving numerical methods see¹

Electronic Implementation

This section shows how to implement a numerical algorithm in a circuit design. For example if we start with Simpson's Rule equation (10), we can first modify it to be causal. This means that we can deal with indices $n, n-1$ etc so that at time 0 we use the index n (i.e. the system is not operating before time $t=0$). We do this by changing the indexing in equation (delaying by 1 sample) (10).

$$\int_{-h}^{+h} f(x_{n-1}) dx = \frac{h}{3} [f_n + 4f_{n-1} + f_{n-2}] \quad (11)$$

¹ Steve E. Koonin, *Computational Physics*, Addison-Wesley, pp 2-6 (1986)

The block diagram is shown below in Figure 1

Block Diagram

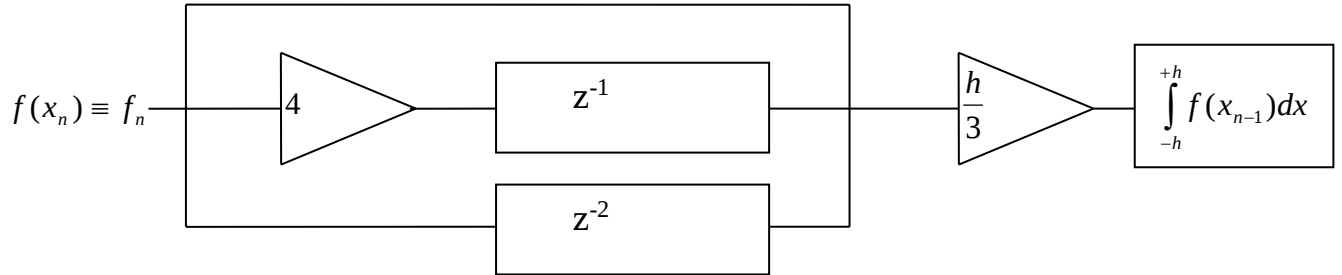


Figure 1

This is shown as a system that can be implemented in the digital domain. The z^{-1} and z^{-2} represent delays of 1 and 2 samples respectively. They could be implemented with digital electronics, analog electronics or theoretically other mechanical or electrical systems which provide a delay equivalent to one sample in time and gain elements.