§4.1 Numerical Differentiation

Recall

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

Suppose that $x_0, x_1 \in [a,b]$ with $h = x_1 - x_0$, then the Lagrange Polynomial for f is

$$f(x) = P_1(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))$$

provided f is $C^2[a,b]$, where

$$P_1(x) = \frac{f(x_0)(x-x_0-h)}{-h} + \frac{f(x_0+h)(x-x_0)}{h}$$

and $\xi(x)$ is between x_0 and x_1. Then differentiating:

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

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

$$+ \frac{(x-x_0)(x-x_0-h)}{2} \underbrace{\frac{d}{dx}\left[f''(\xi(x))\right]}_{\text{we don't know this}}$$

But when $x = x_0$:

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

So for small h,

$$\left| f'(x_0) - \frac{f(x_0+h)-f(x_0)}{h} \right| \le \frac{M|h|}{2}$$

where $|f''(x)| \le M$ for x between x_0 and x_0+h.

Forward Difference Formula

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

for $h>0$, with error bounded by $\frac{Mh}{2}$, and $|f''(x)| \le M$ for x between x_0 and x_0+h.

If $h<0$ then it is called a backward difference formula.

Taylor Polynomials:

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2!}(x-x_0)^2 + \dots$$

So

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} + \mathcal{O}(h)$$

Now look at $(h>0)$

$$\begin{aligned} f(x_0+h) - f(x_0-h) &= \left(f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2!}h^2 + \frac{f'''(x_0)}{3!}h^3 + \dots\right) \\ &\quad - \left(f(x_0) - f'(x_0)h + \frac{f''(x_0)}{2!}h^2 - \frac{f'''(x_0)}{3!}h^3 + \dots\right) \\ &= 2h f'(x_0) + \frac{2}{3!} f'''(x_0) h^3 + \dots \end{aligned}$$

So Centered Difference formula

$$f'(x_0) = \frac{f(x_0+h)-f(x_0-h)}{2h} + \mathcal{O}(h^3)$$

Three-point Endpoint Formula:

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

where ξ_0 is between x_0 and x_0+2h.

Three-point Midpoint Formula:

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

Where ξ_1 is between x_0-h and x_0+h.

Look on page 176 for 5-point formulas

Second Derivative Formulas

Midpoint:

$$f''(x_0) = \frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2} - \frac{h^2}{12}f^{(4)}(\xi)$$

Where ξ is between x_0-h and x_0+h.