

MAT360 Section Summary: 4.1

Numerical Differentiation

1. Summary

In this section we use various schemes for approximating derivatives, using discrete points, starting from the first-order divided difference approximation

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

This is a **two-point** formula, for the approximation, relying on points x_0 and $x_0 + h$. If we can use two points, can't we use three to get even better approximations? Of course we can!

2. Definitions

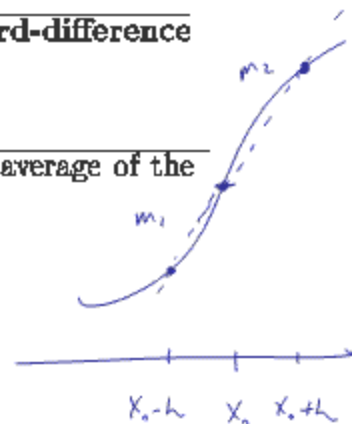
- Given

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

forward-difference formula: $h > 0$; **backward-difference formula:** $h < 0$.

- **centered-difference formula:** works out to the average of the forward- and backward- difference formulas:

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



3. Theorems/Formulas

But what error are we making in that approximation? Well, if f is twice differentiable, then this approximation will fall out of the Lagrange interpolating polynomial and its error term. Consider two points x_0

and x_1 , and the linear Lagrange interpolating polynomial. Define $h = x_1 - x_0$. Then

$$f(x) = P_{0,1}(x) + f''(\xi(x)) \frac{(x-x_0)(x-x_1)}{2!}$$

Then

$$f'(x) = P'_{0,1}(x) + \frac{d}{dx} f''(\xi(x)) \frac{(x-x_0)(x-x_1)}{2!} + f''(\xi(x)) \frac{d}{dx} \left[\frac{(x-x_0)(x-x_1)}{2!} \right]$$

The Newton form of the interpolating polynomial (which is equivalent to the Lagrange interpolating polynomial, remember!) gives us the derivative as the divided difference, and then we have to use the product rule to produce the mess with the rest:

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

When $x = x_0$ we get some nice simplification: we have that

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

so, in general, the forward (or backward) difference approximations have errors that satisfy

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

where $M > 0$ is a bound on the size of the second derivative on the interval $[x_0, x_1]$.

4. Properties/Tricks/Hints/Etc.

We can get the error bound for the centered-difference formula using Taylor series quite easily, provided f is thrice-differentiable:

$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{3!} f'''(\xi(x_0))$$

$$f(x_0) = f(x_0)$$

← The Taylor series gets zero weight in the centered formula.

and
$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{3!} f'''(\xi(x_0))$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{3!} f'''(\phi(x_0))$$

Then the centered-difference formula yields

$$\frac{f(x_0 + h) - f(x_0 - h)}{2h} = f'(x_0) + \frac{h^2}{2 \cdot 3!} (f'''(\xi(x_0)) + f'''(\phi(x_0)))$$

and, provided f''' is continuous, we can find a $\psi(x_0) \in [x_0 - h, x_0 + h]$ such that

$$f'''(\psi(x_0)) = \frac{(f'''(\xi(x_0)) + f'''(\phi(x_0)))}{2}$$

so that

$$\frac{f'(x_0)}{f'(x_0)} = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - f^{(3)}(\psi(x_0)) \frac{h^2}{6}$$

Marvellous! Don't you love that Taylor formula?