MACM 316 Lecture 26 - Chapter 4

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Key Takeaways from this Lecture

Be aware that most of what we did in this chapter is looking over formulas for approximating derivatives. So this entire notes package is just math. The key takeaways are just point forms of what we went over.

1. Numerical Differentiation (1)
   (a) We approximate derivatives using interpolation of easier functions (**ex.** Lagrange polynomials)
   (b) Simplest case: using two points to approximate the first derivative
   (c) The **Forward Difference Formula** (for $h > 0$) and **Backward Difference Formula** (for $h < 0$) are basic numerical differentiation methods (1)
2. More General Approximation Formulas (1.1)
   (a) Using $(n + 1)$-point formulas, we get more accurate derivative approximations
   (b) These formulas all follow from differentiating Lagrange polynomials
   (c) Three, five and higher-order point formulas are commonly used
   (d) Formula reference: (**??**). The error term depends on the highest derivative of $f(x)$ and the spacing of the nodes.
3. Equally Spaced Three-Point Formulas (1.1.2)

(a) When the points are evenly spaced, the formulas for approximating derivatives become (2), (3) and (4)

(b) These three formulas correspond to

   i. Forward Difference (uses two points ahead)

   ii. Centered Difference (uses one point in front and one point behind)

   iii. Backward Difference (uses two points behind)

(c) Check out Example 1 (Section 1.1.3)

4. Second Derivative Approximation (1.1.4)

   (a) We approximate $f''(x)$ by using function values at three points.

   (b) The formulas are derived using Taylor series expansion: (5)

5. Remarks on Error 1.1.5

   (a) **Small h leads to large roundoff errors.**

   (b) Since numerical differentiation involves dividing by h and higher orders of h, extremely small h values can exaggerate computational errors.

   (c) Typically, beyond $h \approx 10^{-6}$, roundoff errors dominate the calculation.

6. Richardson's Extrapolation 2

   (a) If the error depends on some parameter (such as the step size h) and the dependency of the error is predictable (we know the erroe behaviour), we can extrapolate to obtain more accurate approximations.

   (b) We use multiple approximations at different step sizes and **combine them to cancel error terms**.

   (c) There's a step by step process here: (6), (7), (8), (9), (10), (11)

   (d) This process gives increasing accuracy with each step.

7. Final Remarks

   (a) Numerical differentiation can **amplify errors**, so careful step-size selection is crucial.

(b) Centered difference methods are generally more accurate than forward or backward differences.

(c) **Richardson's Extrapolation** is a systematic way to improve accuracy.

(d) In numerical integration (covered in a later part of this chapter), we will integrate the Lagrange polynomial instead of differentiating it.

8. Also check out Random Stuff Steve said during lecture 2.1

1 Numerical Differentiation (C4*1-17.1)

We also need to approximate the derivatives of functions. One approach is to differentiate Lagrange polynomial approximations.

Suppose $x_0, x \in (a, b)$ and $f \in C^2[a, b]$.

Now

$$\begin{aligned} f(x) &= P_{0,1}(x) + \frac{1}{2!}(x - x_0)(x - x_1) f''(\xi(x)) \\ &= \frac{f(x_0)(x - x_1)}{x_0 - x_1} + \frac{f(x_1)(x - x_0)}{x_1 - x_0} + \frac{(x - x_0)(x - x_1)}{2!} f''(\xi(x)) \\ &\text{where } \xi(x) \in [a, b] \end{aligned}$$

Now differentiate:

$$\begin{aligned} f'(x) &= \frac{f(x_1) - f(x_0)}{x_1 - x_0} + D_x \left[\frac{(x - x_0)(x - x_1)}{2!} f''(\xi(x)) \right] \\ &= \frac{f(x_1) - f(x_0)}{x_1 - x_0} + \frac{2(x - x_0)(x - x_1)}{2} f''(\xi(x)) \\ &\quad + \frac{(x - x_0)(x - x_1)}{2} D_x \left(f''(\xi(x)) \right) \end{aligned}$$

We only care about the derivatives at the nodes x_0, x_1. The last error term becomes zero.

For example, at $x = x_0$,

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{x_1 - x_0} - \frac{(x_0 - x_1)}{2} f''(\xi).$$

Typically, we set $x_1 = x_0 + h$, then

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi(x_0)) \tag{1}$$

This is known as a forward difference formula if $h > 0$ and a backward difference formula if $h < 0$. We can derive more general approximation formulas:

1.1 More General Approximation Formulas (17.3)

Suppose $x_0, x_1, \ldots x_n \in (a, b)$ and $f \in C^{n+1}[a, b]$. Now

$$\begin{aligned} f(x) = & \sum_{k=0}^{n} f(x_k) L_k(x) \\ & + \frac{(x - x_0) \ldots (x - x_n)}{(n+1)!} f^{(n+1)}(\xi(x)) \end{aligned}$$

for some $\xi(x) \in [a, b]$

Differentiate and evaluate at $x = x_j$:

$$\begin{aligned} f'(x_j) = & \sum_{k=0}^{n} f(x_k) L_k'(x_j) \\ & + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{k=0;k\neq j}^{n} (x_j - x_k) \end{aligned}$$

This is an $(n + 1)$ point formula for $f'(x_j)$ since we use the $(n + 1)$ values $f(x_k); k = 0, \ldots, n$. Two, three and five point formulas are hte most commonly used formulas.

1.1.1 Three Point Formulas (17.4)

Consider 3 point formulas with x_0, x_1 and x_2.

Given $n = 2$:

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

Taking the derivative:

$$L_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}$$

Similarly,

$$L_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}$$

$$L_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

and

$$\begin{aligned}
f'(x_j) = f[x_0] &\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] \\
&+ f[x_1]\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right] \\
&+ f[x_2]\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right] \\
&+ \frac{1}{6} f^{(3)}(\xi_j) \prod_{\substack{k=0 \\ k \neq j}}^{2} (x_j - x_k)
\end{aligned}$$

These simplify considerably when nodes are equally spaced:

1.1.2 Equally Spaced Three Point Formulas (17.5)

Given:

$$x_1 = x_0 + h, \quad x_2 = x_0 + 2h$$

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

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2}f(x_1-h) + \frac{1}{2}f(x_1+h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1) \tag{3}$$

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_2-2h) - 2f(x_2-h) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_2) \tag{4}$$

For convenience, replace x_1 and x_2 by x_0. This gives 3 formulas for approximating $f'(x_0)$.

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

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

$$f'(x_0) = \frac{1}{h}\left[\frac{1}{2}f(x_0-2h) - 2f(x_0-h) + \frac{3}{2}f(x_0)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

Formula 1 uses two points ahead, formula 2 uses one point in front and one point behind, and formula 3 uses two points behind.

1.1.3 Example 1 (17.5.1)

Ex. use the most appropriate three-point formula to determine approximatinos that will complete the following table:

x	$f(x)$	$f'(x)$
1.1	9.025013	
1.2	11.02318	
1.3	13.46374	
1.4	16.44465	

ANSWER: (17.6)

We only have data in $[1.1, 1.4]$, and no data before or after this interval. So, for $f'(1.1)$ we use formula 1. For $f'(1.2)$ we can use formula 2 or formula 1, but since formula 2 has a smaller error, we choose it. We do the same for $f'(1.3)$. For $f'(1.4)$ we use formula 3, since we only have data behind, and no available data ahead.

$$f'(1.1) \approx \frac{1}{2(0.1)}\left[-3f(1.1) + 4f(1.2) - f(1.3)\right] = 17.769705$$

$$f'(1.2) \approx \frac{1}{2(0.1)}\left[f(1.3) - f(1.1)\right] = 22.193635$$

$$f'(1.3) \approx \frac{1}{2(0.1)}\left[f(1.4) - f(1.2)\right] = 27.107350$$

$$f'(1.4) \approx \frac{1}{2(0.1)}\left[f(1.2) - 4f(1.3) + f(1.4)\right] = 32.510850$$

**these are OCR'd through ChatGPT. They may be wrong.*

Notice that at the endpoints we must use one sided difference formulas. In the interior, we used centered differencing. Centered differences often have a smaller error constant when f is smooth, and they require fewer operations to compute, but they cannot be used at the endpoints.

1.1.4 The Second Derivative of f (17.8)

Approximations to higher order derivatives may also be found based on function values. Consider finding the second derivative of f.

$$f(x_0+h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$
$$f(x_0-h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4$$

where $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

Summing:

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{h^4}{24}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right] \quad (5)$$

We assume $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$.

Since $\frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the *intermediate value theorem* implies that there is a number ξ between ξ_1 and ξ_2 such that

$$f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right].$$

Thus,

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{h^4}{24}f^{(4)}(\xi).$$

Therefore,

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0-h) - 2f(x_0) + f(x_0+h)\right] - \frac{h^2}{24}f^{(4)}(\xi).$$

1.1.5 Remarks on Error (17.9)

Notice that all the differentiation formulas divide by some power of h. Division by small numbers tends to exaggerate roundoff error, but this is an effect that cannot be entirely avoided in numerical differentiation. Thus we do not want to take h to be too small because then the roundoff errors will dominate the calculation.

The exact value at which h becomes too small depends on the scaling of your problem and your specific function f. However, for most problems, scaled nicely, you will start to see roundoff errors at around $h = 10^{-6}$.

2 Richardson's Extrapolation (C4*1-17.10)

When the error depends on some parameter such as the step size h and the dependency is predictable, we can often derive higher order accuracy from low order formulas. To illustrate the procedure, assume we have an approximation $N(h)$ to some quantity M. Assume this approximation has an order h truncation error and that we know the expression for the first few terms of the trunction error,

$$M = N(h) + k_1 h + k_2 h^2 + k_3 h^3 + \dots \tag{6}$$

where the k_i's are constants, h is a positive parameter and $N(h)$ is an $O(h)$ approximation to M. We can repeat the calculation with a parameter $\frac{h}{2}$. Now:

$$M = N(\frac{h}{2}) + \frac{k_1}{2} h + \frac{k_2}{4} h^2 + \frac{k_3}{8} h^3 + \dots. \tag{7}$$

We want to obtain a higher order method by using some combination of these results.

Subctracting (6) from twice (7) gives:

$$M = [2N(\frac{h}{2}) - N(h)] + k_2(\frac{h^2}{2} - h^2) + k_3(\frac{h^3}{4} - h^3) + \dots \tag{8}$$

which is an $O(h^2)$ approximation formula for M. For ease of notiation,

$$\text{Let } N_2(h) = 2N(\frac{h}{2}) - N(h).$$

Now

$$M = N_2(h) - \frac{1}{2} k_2 h^2 - \frac{3}{4} k_3 h^3 - \dots \tag{9}$$

We can repeat this calculation with $\frac{h}{2}$:
Now

$$M = N_2(\frac{h}{2}) - \frac{1}{8} k_2 h^2 - \frac{3k^3}{32} h^3 - \dots \tag{10}$$

We want to eliminate the h^2 term. We can do this by subtracting four times (9) from (10), which gives:

$$3M = 4N_2(\frac{h}{2}) - N_2(h) + \frac{3k_3}{8}h^3 + \dots \tag{11}$$

which gives an $O(h^3)$ formula for approximating M.

$$M = N_3(h) + \frac{1}{3}J_3h^3 + \dots$$

where

$$N_3(h) = \frac{4}{3}N_2\left(\frac{h}{2}\right) - \frac{1}{3}N_2(h).$$

Similarly, an $O(h^4)$ approximation can be derived as:

$$N_4(h) = N_3\left(\frac{h}{2}\right) + \frac{N_3(h/2) - N_3(h)}{7}.$$

And an $O(h^5)$ approximation:

$$N_5(h) = N_4\left(\frac{h}{2}\right) + \frac{N_4(h/2) - N_4(h)}{15}.$$

Generally, if M can be written as:

$$M = N(h) + \sum_{j=1}^{m-1} K_j h^j + O(h^m),$$

then for each $j = 2, 3, \dots, m$, we have an $O(h^j)$ approximation of the form:

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}\left(\frac{h}{2}\right) - N_{j-1}(h)}{2^{j-1} - 1}.$$

2.1 More remarks - things that Steve said during lecture

Chapter 4 also considers numerical integration. We know how to integrate polynomials, so we can just integrate the lagrange polynomial and call it a day.