CMPS251 - Assignment 7

Kinan Dak Al Bab, 201205052

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1 Third derivative approximation

1.1 Question

Derive the following expression for computing the third derivative and its error term (for the error term, derive both the constant and the exponent of the leading term)

$$f```(x) \approx \frac{1}{2h^2}[f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)]$$

1.2 Solution

From Taylor we have:

$$f(x+h) = f(x) + f`(x)h + \frac{f``(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}}{4!}h^4 + O(h^5) \quad (1)$$

$$f(x-h) = f(x) - f`(x)h + \frac{f``(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}}{4!}h^4 + O(h^5) \quad (2)$$

$$f(x+2h) = f(x) + f`(x)2h + \frac{f``(x)}{2!}4h^2 + \frac{f'''(x)}{3!}8h^3 + \frac{f^{(4)}}{4!}16h^4 + O(h^5) \quad (3)$$

$$f(x-2h) = f(x) - f`(x)2h + \frac{f``(x)}{2!}4h^2 - \frac{f'''(x)}{3!}8h^3 + \frac{f^{(4)}}{4!}16h^4 + O(h^5) \quad (4)$$

Now we multiply 1 by -2, 2 by 2, 3 by 1, and 4 by -1 and we sum the resulting equations up.

$$-2f(x+h) + 2f(x-h) + f(x+2h) - f(x-2h) = \frac{12}{3!}f```(x)h^3 + O(h^5) \quad (5)$$

The h^4 term zeroed out when we summed the equations (it got a co-efficient equals to zero). so we have to expand the $O(h^5)$ in all 4 original equations then use the same linear transformation.

$$-2 \times \frac{f^{(5)}(x)}{5!}h^5 + 2 \times (-\frac{f^{(5)}(x)}{5!}h^5) + 1 \times \frac{f^{(5)}(x)}{5!}(2h)^5 - 1 \times (-\frac{f^{(5)}(x)}{5!}(2h)^5)$$

$$= (-4 + 2^6) \times \frac{f^{(5)}(x)}{5!} h^5 = \frac{60}{5!} \times f^{(5)}(x) h^5 = \frac{1}{2} \times f^{(5)}(x) h^5$$

So Now, equation 5 looks like this:

$$-2f(x+h)+2f(x-h)+f(x+2h)-f(x-2h) = \frac{12}{3!} f'''(x) h^3 + \frac{1}{2} \times f^{(5)}(x) h^5 + O(h^6)$$

$$\frac{12}{6} f'''(x) h^3 = -2f(x+h)+2f(x-h)+f(x+2h)-f(x-2h) - \frac{1}{2} f^{(5)}(x) h^5 + O(h^6)$$

$$f'''(x) = \frac{1}{2h^3}[-2f(x+h)+2f(x-h)+f(x+2h)-f(x-2h)] - \frac{1}{2h^3} \times \frac{1}{2} f^{(5)}(x) h^5 + O(h^6)$$

$$f'''(x) = \frac{1}{2h^3}[-2f(x+h)+2f(x-h)+f(x+2h)-f(x-2h)] - \frac{f^{(5)(x)}}{4} \times h^2 + O(h^6)$$

$\therefore$ The leading term is $-\frac{f^{(5)(x)}}{4} \times h^2$, The constant is $-\frac{f^{(5)(x)}}{4}$ so it depends on the fifth derivative of the function, and the power is 2. The error behaves in order of $O(h^2)$.

2 Errors in finite difference approximations

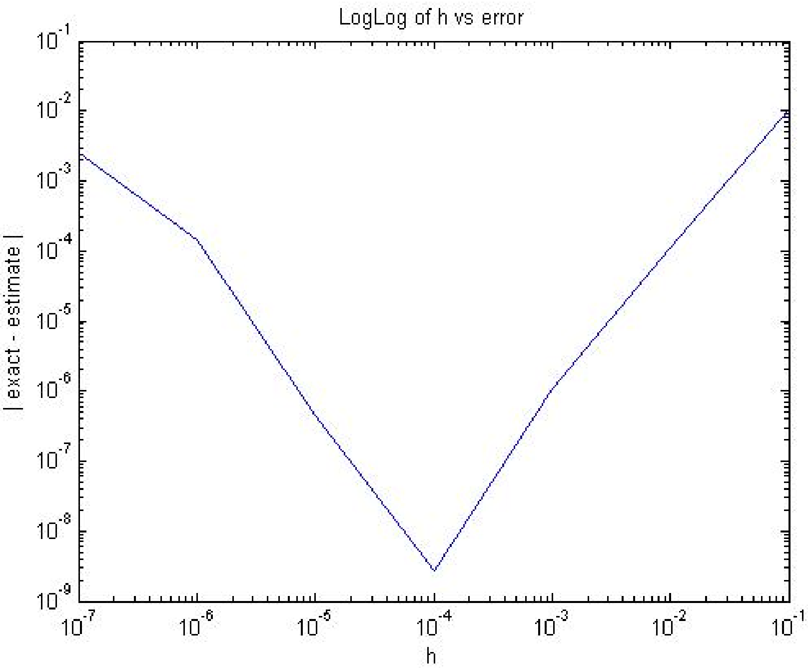
2.1 Question

Generate an appropriate error-vs-h log-log plot to verify the second order accuracy.

2.2 Code

```
format long
syms x;
f = exp(x) * sin(3*x);
x0 = 0.4;

exact = subs(diff(diff(f)), x0);
for i = 1:7
    h(i) = 10^(-i);

    est = (subs(f, x0 - h(i)) - 2*subs(f, x0) + subs(f, x0 + ...
        h(i))) /  h(i)^2;
    err(i) = abs(exact - est);
end

loglog(h, err);
title('LogLog of h vs error');
ylabel('| exact - estimate |');
xlabel(' h ');

first_slope = (log(err(3)) - log(err(1)))/(log(h(3)) - log(h(1)))
second_slope = (log(err(4)) - log(err(1)))/(log(h(4)) - log(h(1)))
```

2.3 Plot and Output




```
first_slope =

   1.994396301942911 % slope between h=10^-1 and h=10^-3


second_slope =

   2.596623701802676 % slope between h=10^-3 and h=10^-4
```

2.4 Comment

- We got nearly the exact expected slope (2) between $h = 10^{-1} andh = 10^{-3}$, indicating $O(h^2)$ behavior.
- Surprisingly, between $h = 10^{-3} andh = 10^{-4}$ the slope was nearly 2.5, better than expected ($h = 10^{-4}$ gives optimal results).
- For $h < 10^{-5}$ The error behaves weirdly and increases, that is due to the fact that the floating point errors take over most of the error, and as we make the h smaller and smaller, these errors become more and more visible (due to the h^2 in the denominator).
- Also it is expected that for $h > 10^{-1}$ The error wouldn't behave in $O(h^2)$ because the other powers of h become important and un-negligible for bigger h.

3 Richardsonś extrapolation (Solving While running out of time)

3.1 Problem 4 - Solution (Didn't Understand the question very much)

From Taylor We Know That:

$$f(x0+h) = f(x0) + f'(x0)h + \frac{f''(x0)}{2}h^2 + O(h^3)$$
$$f(x0-h) = f(x0) - f'(x0)h + \frac{f''(x0)}{2}h^2 + O(h^3)$$

Add Both Equations (Odd-Powered Terms Cancel Out):

$$f(x0+h) + f(x0-h) = 2f(x0) + f''(x0)h^2 + O(h^4)$$
$$\therefore f''(x0) = \frac{f(x0+h) - 2f(x0) + f(x0-h)}{h^2} + C \times h^2 + O(h^4)$$

Similarly for $2h$ we get:

$$f''(x0) = \frac{f(x0+2h) - 2f(x0) + f(x0-2h)}{4h^2} + 4C \times h^2 + O(h^4)$$

Now Multiply The first of these two equations by 4 and subtract the second from it, we get: a formula that approximates the second derivative with an error in order of $O(h^4)$.

3.2 Problem 5 - Solution

We know that each of the given equations approximate the second derivative to $O(h^2)$. Further more this big O can be expanded into $(C, 4C, 9C) \times h^2 + (C', 8C', 27C') \times h^4 + O(h^6)$ For each of the equations respectively.

What we need to do is find a linear combination of 2 of these equations with the constants expanded that would sum these constants up to zero, to get rid of the leading h^2 and get something in the order of $O(h^4)$We need to do the same thing again for another two equations from them and we would get something in the order of $O(h^4)$ as well.

Now we expand the constants in these two formulas and derive a linear combination that would eliminate it, and then we would get something in the order of $O(h^6)$.

Take the first two equations, an obvious linear combination would be: $4 \times EQ_1 - EQ_2$ which will yield a formula with $-4C'$ as constant for the leading h^4.

Take the first and last equations, an obvious linear combination would be: $9 \times EQ_1 - EQ_3$ which will yield a formula with $-18C'$ as constant for the leading h^4.

Now we take the new two formulas and apply this linear combination: $\frac{18}{4} \times NEQ_1 - NEQ_2$. That will yield a formula with no h^4 term, (by construction in a sense). Leaving the leading term to be of the order of h^6. remember, the odd power terms canceled out when deriving the first given 3-formulas.

3.3 Problem 6 - Solution

We know that each of the given equations approximate the second derivative to $O(h^2)$. Further more this big O can be expanded into $(C, 4C, 9C) \times h^2 + O(h^4)$ For each of the equations respectively.

What we need to do is find a linear combination of these 3 equations with the constants expanded that would sum these constants up to zero, to get rid of the leading h^2 and get something in the order of $O(h^4)$.

Such a linear combination would be: $EQ_3 - (EQ_1 + 2 \times EQ_2)$ which would result in:

$$-2f''(x0) = \frac{1}{9h^2}(f(x0-3h) - 2f(x0) + f(x0+3h))$$
$$-\frac{1}{h^2}(f(x0-h) - 2f(x0) + f(x0+h))$$
$$-\frac{1}{h^2}(f(x0-2h) - 2f(x0) + f(x0+2h))$$
$$+10C'h^4 + O(h^6)$$

I am assuming that the question requires us to use the three equations, we could have used any two equations of these equation without the third equation to get an error in order of h^4, which would have required us to do less function evaluations.

4 Numerical differentiation via an interpolating polynomial

4.1 Question

Another way to obtain approximations of derivatives is by fitting an interpolating polynomial in the neighborhood of interest and using the derivatives of the polynomial as the approximation.

For example, in order to obtain an approximation of the second derivative at x_0, we can use a quadratic interpolating polynomial at 3 points $x_0 - h_1, x_0, and x_0 + h_2$. (Notice the unequal spacing around x_0).

- Write the Newton form of this polynomial
- Differentiate it twice to obtain an expression that approximate $f''(x_0)$
- Using the error in the interpolating polynomial, derive the order of accuracy of your approximation of the second derivative.

4.2 Solution

Part 1: Name the original function f, We interpolate it using newton form polynomial on the given points. the interpolating polynomial is the following:

$$p(x) = f(x_0-h_1)+f[x_0-h_1, x_0](x-(x_0-h_1))+f[x_0-h_1, x_0, x_0+h_2](x-(x_0-h_1))(x-x_0)$$

Part 2: Now We differentiate $p(x)$ twice to get the derivative we want:

$$p'(x) = f[x_0-h_1, x_0]+f[x_0-h_1, x_0, x_0+h_2](x-(x_0-h_1))+f[x_0-h_1, x_0, x_0+h_2](x-x_0)$$

$$p''(x) = f[x_0-h_1, x_0, x_0+h_2] + f[x_0-h_1, x_0, x_0+h_2] = 2f[x_0-h_1, x_0, x_0+h_2]$$

So the second derivative is a constant, which makes sense given that the interpolating polynomial is of degree 2. Furthermore we Know how to calculate this divided difference:

$$f[x_0 - h_1, x_0, x_0 + h_2] = \frac{\frac{f(x_2)-f(x_1)}{x_2-x_1} - \frac{f(x_1)-f(x_0)}{x_1-x_0}}{x_2 - x_0}$$

Where $x_1 = x_0 - h_1, x_2 = x_0, x_3 = x_0 + h_2$

Part 3: We know from Newton Interpolation that:

$$f(x) = p(x) + \frac{f^{(n+1)}(\zeta)}{(n+1)!} \times \prod_{i=1}^{n}(x - x_i)$$

Let $\frac{f^{(n+1)}(\zeta)}{(n+1)!} = C$, We differentiate twice:

$$f'(x) = p'(x)+(x-x_0)(x-(x_0+h_2))C+(x-(x_0-h_1))(x-(x_0+h_2)C+(x-(x_0-h_1))(x-x_0)C$$

$$f''(x) = p''(x) + 2C(x - (x_0 - h_1))(x - x_0)(x - (x_0 + h_2))$$

So the error is:

$$2C(x-(x_0-h_1))(x-x_0)(x-(x_0+h_2)) = (6x-2(x_0-h_1)-2x_0-2(x_0+h_2))C$$

We can put an upper bound on the error by putting an upper bound on C, which is by taking C to be the maximum value of the $n+1$ derivative in the range $[x_0 - h_1, x_0 + h_2]$ divided by $(n+1)!$.

The error is in order $O(x)$. so it behaves linearly.