Scientific Computation HW1

Michael Nameika

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Exercise 1.1 *(derivation of finite difference formula)*

Determine the interpolating polynomial $p(x)$ discussed in Example 1.3 and verify that evaluation $p'(\bar{x})$ gives equation (1.11).

Since we are given three points $x_0 = \bar{x} - 2h$, $x_1 = \bar{x} - h$, and $x_2 = \bar{x}$, the quadratic interpolant for x_0, x_1, x_2, $p(x)$ will be unique. That is, we may use any interpolating polynomial we like. I will be using a Lagrange interpolating polynomial. Recall that a quadratic Lagrange interpolating polynomial is given by

$$p(x) = y_0 \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} + y_1 \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} + y_2 \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

where y_0, y_1, y_2 are the values we wish to interpolate and x_0, x_1, x_2 are the associated x values.
Using this formula, we find the following interpolating polynomial:

$$p(x) = u(\bar{x} - 2h) \frac{(x - (\bar{x} - h))(x - \bar{x})}{((\bar{x} - 2h) - (\bar{x} - h))((\bar{x} - 2h) - \bar{x})} + u(\bar{x} - h) \frac{(x - (\bar{x} - 2h))(x - \bar{x})}{((\bar{x} - h) - (\bar{x} - 2h))((\bar{x} - h) - \bar{x})} + \cdots$$

$$\cdots + u(\bar{x}) \frac{(x - (\bar{x} - 2h))(x - (\bar{x} - h))}{((\bar{x} - (\bar{x} - 2h))(\bar{x} - (\bar{x} - h))}$$

Simplifying and expanding, we find

$$p(x) = u(\bar{x} - 2h) \frac{x^2 - (\bar{x} - h)x - x\bar{x} + \bar{x}(\bar{x} - h)}{2h^2} - u(\bar{x} - h) \frac{x^2 - x(\bar{x} - 2h) - \bar{x}x + \bar{x}(\bar{x} - 2h)}{h^2} + \cdots$$

$$\cdots + u(\bar{x}) \frac{x^2 - x(\bar{x} - 2h) - \bar{x}x + \bar{x}(\bar{x} - 2h)}{2h^2}$$

Now, we need to find the derivative of $p(x)$ and evaluate at $x = \bar{x}$. Differentiating the $p(x)$ above and simplifying, we find

$$p'(x) = u(\bar{x} - 2h) \frac{2x + h - 2\bar{x}}{2h^2} - u(\bar{x} - h) \frac{2x + 2h - 2\bar{x}}{h^2} + u(\bar{x}) \frac{2x + 3h - 2\bar{x}}{2h^2}$$

Plugging in $x = \bar{x}$ into the above equation for $p'(x)$, we find

$$p'(\bar{x}) = \frac{1}{2h}(u(\bar{x} - 2h) - 4u(\bar{x} - h) + 3u(\bar{x}))$$

Which is what we wished to show.

Exercise 1.2 *(use of* `fdstencil`*)*

(a) Use the method of undetermined coefficients to set up the 5×5 Vandermonde system that would determine a fourth-order accurate finite difference approximation to $u''(x)$ based on 5 equally spaced points,

$$u''(x) = c_{-2}u(x-2h) + c_{-1}u(x-h) + c_0u(x) + c_1u(x+h) + c_2u(x+2h) + O(h^4).$$

We wish to set up a 5×5 Vandermonde matrix to determine a fourth order accurate centered difference approximation for $u''(x)$ with 5 equally spaced points, $x_0 = \bar{x} - 2h$, $x_1 = \bar{x} - h$, $x_2 = \bar{x}$, $x_3 = \bar{x} + h$, $x_4 = \bar{x} + 2h$. To begin, let's expand $u(x)$ around the above 5 points:

$$u(\bar{x}-2h) = u(\bar{x}) - 2hu'(\bar{x}) + \frac{(2h)^2}{2}u''(\bar{x}) - \frac{(2h)^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u''''(\bar{x}) + \mathcal{O}(h^5)$$

$$u(\bar{x}-h) = u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2!}u''(\bar{x}) - \frac{h^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u''''(\bar{x}) + \mathcal{O}(h^5)$$

$$u(\bar{x}) = u(\bar{x})$$

$$u(\bar{x}+h) = u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2!}u''(\bar{x}) + \frac{h^3}{3!}u'''(\bar{x}) + \frac{h^4}{4!}u''''(\bar{x}) + \mathcal{O}(h^5)$$

$$u(\bar{x}+2h) = u(\bar{x}) + 2hu'(\bar{x}) + \frac{(2h)^2}{2!}u''(\bar{x}) + \frac{(2h)^3}{3!}u'''(\bar{x}) + \frac{(2h)^4}{4!}u''''(\bar{x}) + \mathcal{O}(h^5)$$

Multiplying the above equations by c_{-2}, c_{-1}, c_0, c_1, c_2 respectively, and summing them up, we find the following five equations to solve for the second derivative

$$c_{-2} + c_{-1} + c_0 + c_1 + c_2 = 0$$

$$-2hc_{-2} - hc_{-1} + hc_1 + 2hc_2 = 0$$

$$\frac{(2h)^2}{2!}c_{-2} + \frac{h^2}{2!}c_{-1} + \frac{h^2}{2!}c_1 + \frac{(2h)^2}{2!}c_2 = 1$$

$$-\frac{(2h)^3}{3!}c_{-2} - \frac{h^3}{3!}c_{-1} + \frac{h^3}{3!}c_1 + \frac{(2h)^3}{3!}c_2 = 0$$

$$\frac{(2h)^4}{4!}c_{-2} + \frac{h^4}{4!}c_{-1} + \frac{h^4}{4!}c_1 + \frac{(2h)^4}{4!} = 0$$

Writing as a matrix system, we get

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ -2h & -h & 0 & h & 2h \\ \frac{(2h)^2}{2!} & \frac{h^2}{2!} & 0 & \frac{h^2}{2!} & \frac{(2h)^2}{2!} \\ -\frac{(2h)^3}{3!} & -\frac{h^3}{3!} & 0 & \frac{h^3}{3!} & \frac{(2h)^3}{3!} \\ \frac{(2h)^4}{4!} & \frac{h^4}{4!} & 0 & \frac{h^4}{4!} & \frac{(2h)^4}{4!} \end{bmatrix} \begin{bmatrix} c_{-2} \\ c_{-1} \\ c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

Plugging the system into MATLAB and solving, we find

$$\begin{bmatrix} c_{-2} \\ c_{-1} \\ c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{12h^2} \\ \frac{4}{3h^2} \\ -\frac{5}{2h^2} \\ \frac{4}{3h^2} \\ -\frac{1}{12h^2} \end{bmatrix}$$

We wish to show that these coefficients give an $\mathcal{O}(h^4)$ approximation. From the Taylor expansion at the beginning of the problem, we expanded to $\mathcal{O}(h^5)$ and since the coefficients have a $\frac{1}{h^2}$ term, this suggests that our method is $\mathcal{O}(h^3)$. However, including the fifth order terms for the Taylor expansion gives us the following equation:

$$-\frac{1}{12h^2}\frac{(-2h)^5}{5!} + \frac{4}{3h^2}\frac{(-h)^5}{5!} + \frac{4}{3h^2}\frac{h^5}{5!} - \frac{1}{12h^2}\frac{(2h)^5}{5!} \\ = 0$$

So our method will return an $\mathcal{O}(h^4)$ approximation.

(b) Compute the coefficients using the MATLAB code `fdstencil.m` available from the website, and check that they satisfy the system you determined in part (a).

Using the fdstencil.m script, we find the following coefficients

```
The derivative u^(2) of u at x0 is approximated by

          1/h^2 * [
                     -8.333333333333333e-02 * u(x0-2*h) +
                      1.333333333333333e+00 * u(x0-1*h) +
                     -2.500000000000000e+00 * u(x0) +
                      1.333333333333333e+00 * u(x0+1*h) +
                     -8.333333333333333e-02 * u(x0+2*h) ]

For smooth u,
       Error = 0 * h^3*u^(5) + -0.0111111 * h^4*u^(6) + ...
```

Which are exactly the coefficients given by the Vandermonde system in part a).

(c) Test this finite difference formula to approximate $u''(1)$ for $u(x) = \sin(2x)$ with values of h from the array `hvals = logspace(-1, -4, 13)`. Make a table of the error vs. h for several values of h and compare against the predicted error from the leading term of the expression printed by `fdstencil`. You may want to look at the m-file `chap1example1.m` for guidance on how to make such a table.

Also produce a log-log plot of the absolute value of the error vs. h.

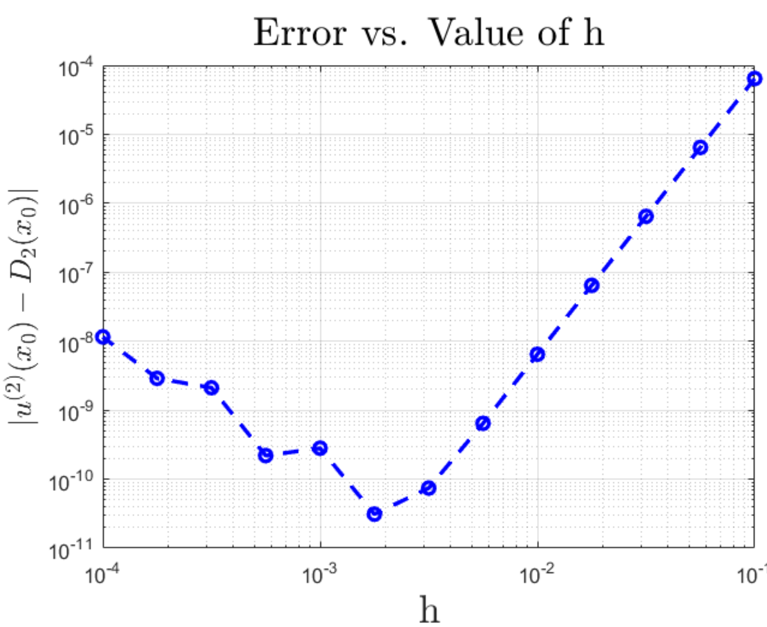
You should observe the predicted accuracy for larger values of h. For smaller values, numerical cancellation in computing the linear combination of u values impacts the accuracy observed.

For this problem, denote the approximation for the second derivative by $D_2(x)$. Using the stencilScript.m code I wrote (see attached m file), we find the following table for error versus h values:

h	Error	Max Predicted Error
1.0000e-01	6.4431e-05	7.1111e-05
5.6234e-02	6.4588e-06	7.1111e-06
3.1623e-02	6.4638e-07	7.1111e-07
1.7783e-02	6.4654e-08	7.1111e-08
1.0000e-02	6.4630e-09	7.1111e-09
5.6234e-03	6.4455e-10	7.1111e-10
3.1623e-03	7.4244e-11	7.1111e-11
1.7783e-03	3.1035e-11	7.1111e-12
1.0000e-03	2.8103e-10	7.1111e-13
5.6234e-04	2.1974e-10	7.1111e-14
3.1623e-04	2.1129e-09	7.1111e-15
1.7783e-04	2.8961e-09	7.1111e-16
1.0000e-04	1.1550e-08	7.1111e-17

Notice that the maximum predicted error has the same order of magnitude of the measured error until the value of h drops below approximately 3.16×10^{-3}.

We also find the following loglog plot for the error:



We notice from the above plot that numerical error begins to take over when $h < 3.16 \times 10^{-3}$, as mentioned above.