Richardson’s Extrapolation

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Approximating the Second Derivative

- From last time, we derived that:

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

the truncation error is \( O(h^2) \).

- Further, rounding error analysis predicts rounding errors of size about \( \epsilon/h^2 \).

- Therefore, the smallest total error occurs when \( h \) is about \( \epsilon^{1/4} \) and then the truncation error and the rounding error are each about \( \sqrt{\epsilon} \).

- With machine precision \( \epsilon \approx 10^{-16} \), this means that \( h \) should not be taken to be less than about \( 10^{-4} \).

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In order to actively see the rounding effects in the second order approximation, let us use MATLAB.

You will find the following MATLAB code on the course webpage:

```matlab
f = inline('sin(x)');
fppTrue = inline('-sin(x)');
h = 0.1;
x = pi/3;

fprintf(' h Abs. Error
');
fprintf('========================
');
for i = 1:6
    fpp = (f(x+h) - 2*f(x) + f(x-h))/h^2;
    fprintf('%7.1e %8.1e
',h,abs(fpp-fppTrue(x)))
    h = h/10;
end
```
This MATLAB code produces the following table:

<table>
<thead>
<tr>
<th>h</th>
<th>Abs. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0e-001</td>
<td>7.2e-004</td>
</tr>
<tr>
<td>1.0e-002</td>
<td>7.2e-006</td>
</tr>
<tr>
<td>1.0e-003</td>
<td>7.2e-008</td>
</tr>
<tr>
<td>1.0e-004</td>
<td>3.2e-009</td>
</tr>
<tr>
<td>1.0e-005</td>
<td>3.7e-007</td>
</tr>
<tr>
<td>1.0e-006</td>
<td>5.1e-005</td>
</tr>
</tbody>
</table>
Your Turn

- Download the code `secondDeriv.m` from the course web page.
- Edit the code such that it approximates the second derivative of \( f(x) = x^3 - 2 \times x^2 + x \) at the point \( x = 1 \).
- Again, let your initial \( h = 0.1 \).
- After running the code change \( x \) from \( x = 1 \) to \( x = 1000 \). What do you notice?
Your code should have changed the inline functions to the following:

\[ f = \text{inline}(\texttt{'}x^3 - 2x^2 + x\texttt{'})\];
\[ \text{fppTrue} = \text{inline}(\texttt{'}6x - 4\texttt{')}\);

This MATLAB code produces the following table:

<table>
<thead>
<tr>
<th>h</th>
<th>Abs. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0e-001</td>
<td>7.2e-004</td>
</tr>
<tr>
<td>1.0e-002</td>
<td>7.2e-006</td>
</tr>
<tr>
<td>1.0e-003</td>
<td>7.2e-008</td>
</tr>
<tr>
<td>1.0e-004</td>
<td>3.2e-009</td>
</tr>
<tr>
<td>1.0e-005</td>
<td>3.7e-007</td>
</tr>
<tr>
<td>1.0e-006</td>
<td>5.1e-005</td>
</tr>
</tbody>
</table>

How small \( h \) can be depends on the size of \( x \).
Recognizing Error Behavior

- Last time we also saw that Taylor Series of $f$ about the point $x$ and evaluated at $x + h$ and $x - h$ leads to the central difference formula:

$$f'(x) = \frac{f(x + h) - f(x - h)}{2h} - \frac{h^2}{6} f'''(x_0) - \frac{h^4}{120} f^{(5)}(x_0) - \cdots.$$ 

- This formula describes precisely how the error behaves.
- This information can be exploited to improve the quality of the numerical solution without ever knowing $f'''$, $f^{(5)}$, . . .
- Recall that we have a $O(h^2)$ approximation.
Let us rewrite this in the following form:

\[ f'(x_0) = N(h) - \frac{h^2}{6} f''''(x_0) - \frac{h^4}{120} f^{(5)}(x_0) - \cdots , \]

where \( N(h) = \frac{f(x+h)-f(x-h)}{2h} \).

The key of the process is to now replace \( h \) by \( h/2 \) in this formula.

Complete this step:
Canceling Higher Order Terms

Therefore, you find

\[ f'(x_0) = N \left( \frac{h}{2} \right) - \frac{h^2}{24} f''''(x_0) - \frac{h^4}{1920} f^{(5)}(x_0) - \cdots. \]

Look closely at what we had from before:

\[ f'(x_0) = N(h) - \frac{h^2}{6} f''''(x_0) - \frac{h^4}{120} f^{(5)}(x_0) - \cdots. \]

Careful substraction cancels a higher order term.

\[ 4f'(x_0) = 4N \left( \frac{h}{2} \right) - 4 \frac{h^2}{24} f''''(x_0) - 4 \frac{h^4}{1920} f^{(5)}(x_0) - \cdots \]

\[ -f'(x_0) = -N(h) + \frac{h^2}{6} f''''(x_0) + \frac{h^4}{120} f^{(5)}(x_0) + \cdots \]

\[ 3f'(x_0) = 4N \left( \frac{h}{2} \right) - N(h) + \frac{h^4}{160} f^{(5)}(x_0) + \cdots \]
Thus,

\[ f'(x_0) = N\left(\frac{h}{2}\right) + \frac{N(h/2) - N(h)}{3} + \frac{h^4}{160}f^{(5)}(x_0) + \cdots \]

is a \(O(h^4)\) formula.

Notice what we have done. We took two \(O(h^2)\) approximations and created a \(O(h^4)\) approximation.

We did require, however, that we have functional evaluations at \(h\) and \(h/2\).
Further observations

- Again, we have the $O(h^4)$ approximation:

$$f'(x_0) = N\left(\frac{h}{2}\right) + \frac{N(h/2) - N(h)}{3} + \frac{h^4}{160} f^{(5)}(x_0) + \cdots.$$ 

- This approximation requires roughly twice as much work as the second order centered difference formula.

- However, but the truncation error now decreases much faster with $h$.

- Moreover, the rounding error can be expected to be on the order of $\epsilon/h$, as it was for the centered difference formula, so the greatest accuracy will be achieved for $h^4 \approx \epsilon/h$, or, $h \approx \epsilon^{1/5}$, and then the error will be about $\epsilon^{4/5}$. 

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Example

Consider \( f(x) = x \exp(x) \) with \( x_0 = 2.0 \) and \( h = 0.2 \). Use the central difference formula to the first derivative and Richardson’s Extrapolation to give an approximation of order \( O(h^4) \).

Recall \( N(h) = \frac{f(x + h) - f(x - h)}{2h} \).

Therefore, \( N(0.2) = 22.414160 \).

What do we evaluate next?

\[
N(\quad) = \text{__________________________}
\]
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Recall \( N(h) = \frac{f(x + h) - f(x - h)}{2h} \).

Therefore, \( N(0.2) = 22.414160 \).

What do we evaluate next?

\[ N(\quad) = \quad \]

We find \( N(h/2) = N(0.1) = 22.228786 \).
Therefore, our higher order approximation is
Therefore, our higher order approximation is

\[
f'(x_0) = N\left(\frac{h}{2}\right) + \frac{N(h/2) - N(h)}{3}
\]

\[
= N(0.1) + \frac{N(0.1) - N(0.2)}{3}
\]

\[
= 22.1670.
\]

Note, \(f'(x) = x \exp(x) + \exp(x)\), so \(f'(x) = 22.1671\) to four decimal places.

You should find that from approximations that contain zero decimal places of accuracy we attain an approximation with two decimal places of accuracy with truncation.
This process is known as Richardson’s Extrapolation.

More generally, assume we have a formula \( N(h) \) that approximates an unknown value \( M \) and that
\[
M - N(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots
\]
for some unknown constants \( K_1, K_2, K_3, \ldots \). Note that in this example, the truncation error is \( O(h) \).

Without knowing \( K_1, K_2, K_3, \ldots \) it is possible to produce a higher order approximation as seen in our previous example.

Note, we could use our result from the previous example to produce an approximation of order \( O(h^6) \). To understand this statement more, let us look at an example.
Example from numerical integration

The following data gives approximations to the integral

\[ M = \int_0^\pi \sin x \, dx. \]

\[ N_1(h) = 1.570796, \quad N_1\left(\frac{h}{2}\right) = 1.896119, \quad N_1\left(\frac{h}{4}\right) = 1.974242 \]

Assuming \( M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + K_4 h^8 + O(h^{10}) \)

construct an extrapolation table to determine an order six approximation.

**Solution**

As before, we evaluate our series at \( h \) and \( h/2 \) and get:

\[ M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + K_4 h^8 + O(h^{10}), \quad \text{and} \]

\[ M = N_1(h/2) + K_1 \frac{h^2}{4} + K_2 \frac{h^4}{16} + K_3 \frac{h^6}{64} + K_4 \frac{h^8}{256} + O(h^{10}) \]
Example Continued

Therefore,

\[
4M = 4N_1 \left( \frac{h}{2} \right) + K_1 h^2 + K_2 \frac{h^4}{4} + K_3 \frac{h^6}{16} + \cdots
\]

\[
-M = -N(h) - K_1 h^2 - K_2 h^4 - K_3 \frac{h^6}{16} + \cdots
\]

\[
3M = 4N_1 \left( \frac{h}{2} \right) - N_1(h) + \hat{K}_2 h^4 + \hat{K}_3 h^6 + \cdots
\]

Thus, \( M = N_1 \left( \frac{h}{2} \right) + \frac{N_1 \left( \frac{h}{2} \right) - N_1(h)}{3} + \hat{K}_2 h^4 + \hat{K}_3 h^6. \)

Letting \( N_2 = N_1 \left( \frac{h}{2} \right) + \frac{N_1 \left( \frac{h}{2} \right) - N_1(h)}{3} \) we get

\( M = N_2(h) + \hat{K} h^4 + \hat{K}_3 h^6. \)
Again, \( M = N_2(h) + \hat{K} h^4 + \hat{K}_3 h^6 \).

Therefore, \( M = N_2 \left( \frac{h}{2} \right) + \frac{1}{16} \hat{K}_2 h^4 + \frac{1}{64} \hat{K}_3 h^6 \), which leads to:

\[
16M = 16N_2 \left( \frac{h}{2} \right) + \hat{K}_2 h^4 + \frac{1}{4} \hat{K}_3 h^6 + \cdots
\]

\[
-M = -N_2(h) - \hat{K}_2 h^4 - \hat{K}_3 h^6 + \cdots
\]

\[
15M = 16N_2 \left( \frac{h}{2} \right) - N_2(h) + O(h^6)
\]

Hence, \( M = N_2 \left( \frac{h}{2} \right) + \frac{N_2 \left( \frac{h}{2} \right) - N_2(h)}{15} + O(h^6) \).
Example Continued

In terms of a table, we find:

<table>
<thead>
<tr>
<th>Given</th>
<th>( N_1 \left( \frac{h}{2} \right) + \frac{N_1 \left( \frac{h}{2} \right) - N_1(h)}{3} )</th>
<th>( N_2 \left( \frac{h}{2} \right) + \frac{N_2 \left( \frac{h}{2} \right) - N_2(h)}{15} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_1(h) ) = 1.570796</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( N_1 \left( \frac{h}{2} \right) ) = 1.896119</td>
<td>( N_2(h) = 2.004560 )</td>
<td></td>
</tr>
<tr>
<td>( N_1 \left( \frac{h}{4} \right) ) = 1.974242</td>
<td>( N_2 \left( \frac{h}{2} \right) = 2.000270 )</td>
<td>( 1.999984 )</td>
</tr>
</tbody>
</table>

In the chapter on numerical integration, we see that this is the basis of a Romberg integration.
Take a moment and reflect on the process we just followed.

- We began with $O(h^2)$ approximations for which we knew the Taylor expansion.
- We used our $O(h^2)$ approximations to find $N_2$ which were order $O(h^4)$ and again for which we knew the Taylor expansions.
- Finally, we used the $N_2$ approximations to find an $O(h^6)$ approximation.
- Could we continue this to find an order 8 approximation? It depends – remember that reducing $h$ can lead to round-off error. As long as we don’t hit that threshold, then our computations do not corrupt our Taylor expansion.