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 ϵ/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}.

Numerical Derivatives on MATLAB

- 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:

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

fprintf('   h        Abs. Error\n');
fprintf('=========================\n');
for i = 1:6
    fpp = (f(x+h) - 2*f(x) + f(x-h))/h^2;
    fprintf('%7.1e     %8.1e\n',h,abs(fpp-fppTrue(x)))
    h = h/10;
end
```

Rounding errors in action

This MATLAB code produces the following table:

```
    h         Abs. Error
=========================
1.0e-001      7.2e-004
1.0e-002      7.2e-006
1.0e-003      7.2e-008
1.0e-004      3.2e-009
1.0e-005      3.7e-007
1.0e-006      5.1e-005
```

Your Turn

- Download the code `secondDeriv.m` from the course web page.
- Edit the code such that it approximates the second derivative of $f(x) = x^3 - 2 * x^2 + x$ 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?

Rounding errors again

- Your code should have changed the inline functions to the following:

```
f = inline('x^3 - 2*x^2 + x');
fppTrue = inline('6*x - 4');
```

- This MATLAB code produces the following table:

```
     h          Abs. Error
=========================
1.0e-001      7.2e-004
1.0e-002      7.2e-006
1.0e-003      7.2e-008
1.0e-004      3.2e-009
1.0e-005      3.7e-007
1.0e-006      5.1e-005
```

- 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 $f''', f^{(5)}, \ldots$.
- 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.

$$\begin{array}{rcccccc}
4f'(x_0) = & 4N\left(\frac{h}{2}\right) & - & 4\frac{h^2}{24}f'''(x_0) & - & 4\frac{h^4}{1920}f^{(5)}(x_0) & -\cdots \\
-f'(x_0) = & -N(h) & + & \frac{h^2}{6}f'''(x_0) & + & \frac{h^4}{120}f^{(5)}(x_0) & +\cdots \\
\hline
3f'(x_0) = & 4N\left(\frac{h}{2}\right) - N(h) & & & + & \frac{h^4}{160}f^{(5)}(x_0) & +\cdots
\end{array}$$

A Higher Order Method

- 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 ϵ/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 $\epsilon^{4/5}$.

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 $N(h) = \dfrac{f(x+h) - f(x-h)}{2h}$.
- Therefore, $N(0.2) = 22.414160$.
- What do we evaluate next?

$$N(\qquad) = \underline{\hspace{8cm}}$$

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$$N(\qquad) = \underline{\hspace{10cm}}$$

- We find $N(h/2) = N(0.1) = 22.228786$.

Example cont.

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- In particular, we find the approximation:

$$
\begin{aligned}
f'(x_0) &= N\left(\frac{h}{2}\right) + \frac{N(h/2) - N(h)}{3} \\
&= N(0.1) + \frac{N(0.1) - N(0.2)}{3} \\
&= 22.1670.
\end{aligned}
$$

- 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.

<u>Solution</u> As before, we evaluate our series at h and $h/2$ and get:

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

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

Example Continued

Therefore,

$$\begin{array}{rcl} 4M & = & 4N_1\left(\frac{h}{2}\right) \quad + \quad K_1h^2 + K_2\frac{h^4}{4} + K_3\frac{h^6}{16} + \cdots \\ -M & = & -N(h) \quad - \quad K_1h^2 - K_2h^4 - K_3\frac{h^6}{16} + \cdots \\ \hline 3M & = & 4N_1\left(\frac{h}{2}\right) - N_1(h) \quad + \hat{K}_2h^4 + \hat{K}_3h^6 + \cdots \end{array}$$

Thus, $M = N_1\left(\frac{h}{2}\right) + \frac{N_1\left(\frac{h}{2}\right) - N_1(h)}{3} + \hat{K}_2h^4 + \hat{K}_3h^6.$

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

$M = N_2(h) + \hat{K}h^4 + \hat{K}_3h^6.$

Example Continued[2]

Again, $M = N_2(h) + \hat{K}h^4 + \hat{K}_3h^6$.

Therefore, $M = N_2\left(\frac{h}{2}\right) + \frac{1}{16}\hat{K}_2h^4 + \frac{1}{64}K_3h^6$, which leads to:

$$\begin{array}{rrrrrrrr} 16M = & 16N_2\left(\frac{h}{2}\right) & & + & \hat{K}_2h^4 & + & \frac{1}{4}\hat{K}_3h^6 & + \cdots \\ -M = & -N_2(h) & & - & \hat{K}_2h^4 & - & \hat{K}_3h^6 & + \cdots \\ \hline 15M = & 16N_2\left(\frac{h}{2}\right) & - N_2(h) & & & + & O(h^6) & \end{array}$$

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

In terms of a table, we find:

Given	$N_1\left(\frac{h}{2}\right) + \frac{N_1\left(\frac{h}{2}\right) - N_1(h)}{3}$	$N_2\left(\frac{h}{2}\right) + \frac{N_2\left(\frac{h}{2}\right) - N_2(h)}{15}$
$N_1(h) = 1.570796$		
$N_1\left(\frac{h}{2}\right) = 1.896119$	$N_2(h) = 2.004560$	
$N_1\left(\frac{h}{4}\right) = 1.974242$	$N_2\left(\frac{h}{2}\right) = 2.000270$	1.999984

In the chapter on numerical integration, we see that this is the basis of a Romberg integration.

Example summary

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.