4.3 Estimating Derivatives and Richardson's Extrapolation

Consider the problem of estimating $f'(x)$ given $f(x)$.

Use Taylor series to get

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \dots + \frac{h^n}{n!} f^{(n)}(x) + \dots$$

Rearranging we get

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(x) - \frac{h^2}{6} f'''(x) - \dots$$

or

$$f'(x) = \frac{f(x+h) - f(x)}{h} + E$$

where $E = -h\left[\frac{1}{2} f''(x) + \frac{h}{6} f'''(x) + \dots\right]$

Here E is $O(h)$ and so omitting E introduces a truncation error of $O(h)$.

The <u>Forward difference</u> approximation of $f'(x)$ is

$$\boxed{f'(x) \approx \frac{f(x+h) - f(x)}{h} \qquad \text{error is } O(h)}$$

Using Taylor series for $f(x-h)$ we get

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(x) + \dots$$

The <u>Backward difference</u> approximation of $f'(x)$ is

$$\boxed{f'(x) \approx \frac{f(x) - f(x-h)}{h} \qquad \text{error is } O(h)}$$

We can improve things a bit by using both series.

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f^{iv}(x) + \dots$$
$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f^{iv}(x) - \dots$$

$$f(x+h) - f(x-h) = 2hf'(x) + 2\frac{h^3}{6} f'''(x) + 2\frac{h^5}{5!} f^{(5)}(x) + \dots$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \underbrace{- \frac{h^2}{6} f'''(x) - \frac{h^4}{5!} f^{(5)}(x) - \dots}_{E}$$

Where E is now $O(h^2)$

$$\boxed{\begin{array}{l}\text{The centered difference approximation to } f'(x) \\ \text{is} \\ \qquad f'(x) \simeq \dfrac{f(x+h) - f(x-h)}{2h} \qquad \text{error is } O(h^2)\end{array}}$$

In fact, by cleverly combining Taylor expansions of $f(x)$ at different offsets, we can get approximations of higher orders.

Another approach to improved accuracy is Richardson's Extrapolation.

Write our series for $f'(x)$ as

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + a_2 h^2 + a_4 h^4 + \dots + a_{2k} h^{2k} + \dots$$

and let $\phi(h) = \dfrac{f(x+h) - f(x-h)}{2h}$

So $\quad \phi(h) = f'(x) - a_2 h^2 - a_4 h^4 - \cdots$

Next, compute $\phi(\frac{h}{2})$

$$\phi(\tfrac{h}{2}) = f'(x) - a_2\left(\tfrac{h}{2}\right)^2 - a_4\left(\tfrac{h}{2}\right)^4 - \cdots$$
$$= f'(x) - \tfrac{1}{4}a_2 h^2 - \tfrac{1}{4^2}a_4 h^4 - \cdots - \tfrac{1}{4^k}a_{2k}h^{2k}$$

If we multiply $\phi(\frac{h}{2})$ by 4 and subtract $\phi(h)$ from this we'll eliminate the $a_2 h^2$ term

$$4\phi(\tfrac{h}{2}) - \phi(h) = (4-1)f'(x) + (1-\tfrac{4}{4})a_4h^4 + (1-\tfrac{4}{4^2})a_6h^6 + \cdot$$

So
$$f'(x) = \frac{4\phi(\frac{h}{2}) - \phi(h)}{4-1} - \frac{1-\frac{1}{4}}{4-1}a_4h^4 - \frac{1-\frac{1}{4^2}}{4-1}a_6h^6 - \cdots$$

$$= \frac{4\phi(\frac{h}{2}) - \phi(h)}{3} - \frac{4}{4}\frac{(1-\frac{1}{4})}{(4-1)}a_4h^4 - \frac{16(1-\frac{1}{16})}{16(4-1)}a_6h^6 - \cdots$$

$$= \frac{4\phi(\frac{h}{2}) - \phi(h)}{3} \underbrace{- \frac{1}{4}a_4h^4 - \frac{5}{16}a_6h^6 - \cdots}_{O(h^4)}$$

So, we now have an approximation that is $O(h^4)$ rather than $O(h^2)$

We can repeat this again (and again) to improve our accuracy.

Text sets up

$$D(n,0) = \phi\left(\frac{h}{2^n}\right)$$

and then

$$D(n,m) = \frac{4^m}{4^m-1} D(n,m-1) - \frac{1}{4^m-1} D(n-1,m-1) \qquad 1 \le m \le n$$

which can be rewritten as

add and subtract same quantity.

$$D(n,m) = \frac{4^m-1}{4^m-1} D(n,m-1) + \frac{1}{4^m-1} D(n,m-1) - \frac{1}{4^m-1} D(n-1,m-1)$$

$$D(n,m) = D(n,m-1) + \frac{1}{4^m-1}\left[D(n,m-1) - D(n-1,m-1)\right]$$

$D(0,0)$ is $\phi(h)$

$D(1,0)$ is $\phi(\frac{h}{2})$

$D(1,1)$ is $\dfrac{4\phi(\frac{h}{2}) - \phi(h)}{3}$ our $O(h^4)$ approx.

$D(2,0)$ is $\phi(\frac{h}{4})$

$D(2,2)$ is an $O(h^6)$ approx. . .

Forms a triangle

$$\begin{array}{llll}
D(0,0) & & & \\
D(1,0) & D(1,1) & & \\
D(2,0) & D(2,1) & D(2,2) & \\
D(3,0) & D(3,1) & D(3,2) & D(3,3)
\end{array}$$

```
function d = richardson( f, x, n, h )
  % -------------------------------------------------------------------------
  % Jonathan R. Senning <jonathan.senning@gordon.edu>
  % Gordon College
  % February 9, 1999
  %
  % Usage: D = richardson(@f, x, n, h)
  %
  % Returns:
  %     two-dimensional array of extrapolation values.  The n+1,n+1 value
  %     of this array should be the most accurate.
  %
  % Parameters:
  %     f:      handle of function to find derivative of
  %     x:      value of x to find derivative at
  %     n:      number of levels of extrapolation
  %     h:      initial stepsize
  %
  % This function implements Richardson's Extrapolation to determine an
  % approximation of f'(x) at a particular value of x.
  %
  % Based on an algorithm in "Numerical Mathematics and Computing"
  % 4th Edition, by Cheney and Kincaid, Brooks-Cole, 1999.
  %
  % Note: There are several changes that could be made to make this code
  % more efficient.  However, it follows the algorithm in the text very
  % closely.  The main difference is that arrays in octave start with a
  % subscript of 1 rather than 0.
  % -------------------------------------------------------------------------

  % d(n+1,n+1) will contain the most accurate approximation to f'(x).
  d = zeros( n + 1, n + 1 );
  for i = 1 : n + 1
    d(i,1) = 0.5 * ( f( x + h ) - f( x - h ) ) / h;
    for j = 1 : i - 1
      d(i,j+1) = d(i,j) + ( d(i,j) - d(i-1,j) ) / ( 4^j - 1 );
    end
    h = 0.5 * h;
  end
end
```

```
>> format long
>> function y=f(x); y=exp(-x)*sin(x); end
>> x=0.5, n=7, h=1.0
x =  0.500000000000000
n =  7
h =  1
>> richardson(@f,x,n,h)
ans =

 Columns 1 through 4:

   0.506505149660917   0.000000000000000   0.000000000000000   0.000000000000000
   0.309559875653112   0.243911450983844   0.000000000000000   0.000000000000000
   0.258609908168987   0.241626585674279   0.241474261320308   0.000000000000000
   0.245779279120729   0.241502402771310   0.241494123911112   0.241494439190331
   0.242566020941597   0.241494934881886   0.241494437022591   0.241494441992615
   0.241762359786589   0.241494472734919   0.241494441925121   0.241494442002939
   0.241561422888584   0.241494443922582   0.241494442001760   0.241494442002976
   0.241511187314348   0.241494442122936   0.241494442002960   0.241494442002979

 Columns 5 through 8:

   0.000000000000000   0.000000000000000   0.000000000000000   0.000000000000000
   0.000000000000000   0.000000000000000   0.000000000000000   0.000000000000000
   0.000000000000000   0.000000000000000   0.000000000000000   0.000000000000000
   0.000000000000000   0.000000000000000   0.000000000000000   0.000000000000000
   0.241494442003604   0.000000000000000   0.000000000000000   0.000000000000000
   0.241494442002980   0.241494442002979   0.000000000000000   0.000000000000000
   0.241494442002976   0.241494442002976   0.241494442002976*  0.000000000000000
   0.241494442002979   0.241494442002979   0.241494442002979   0.241494442002979
```

$$f(x) = e^{-x} \sin x$$

$$f'(x) = -e^{-x}\sin x + e^{-x}\cos x$$

$$= e^{-x}(\cos x - \sin x)$$

$$f'(0.5) = 0.24149444200979\ldots$$

* Note: Once we reach the maximum precision of the computer, continued work does not improve the result – infact it may lead to less accurate results.

We can use Taylor Series to find a formula for $f''(x)$.

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f^{(4)}(x) + \cdots$$
$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f^{(4)}(x) + \cdots$$

Adding, we find

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{12} f^{(4)}(x) + \frac{h^6}{360} f^{(6)}(x) + \cdots$$

so

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - h^2 \left[\frac{1}{12} f^{(4)}(x) + \frac{h^4}{360} f^{(6)}(x) + \cdots \right]$$

This gives an $O(h^2)$ approximation for $f''(x)$. We call this approximation a <u>centered difference approximation for $f''(x)$.</u>

Note that a Richardson's extrapolation method could be applied to come up with more accurate approximation at the expense of more function evaluations