LECTURE 5

Numerical Differentiation

We shall now look at the problems related to the calculation of derivatives via numerical methods. Now at first thought, it would seem that a numerical calculation of a derivative would be rather straight-forward. For the very definition of the derivative

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

lends itself immediately to a natural numerical approximation for a derivative:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad , \quad h << 1.$$

It would thus seem that, if we wanted to get an extremely accurate value for the derivative of a function, all we'd have to do is pick a small enough value for h and calculate

$$\frac{f(x+h) - f(x)}{h} \tag{1}$$

Let's see if this really works. Let f be the function $f(x) = \sin(x)$, so that $f'(x) = \cos(x)$. We will calculate $f'(1)$ using the formula above using successively small values of h.

```
f := x -> sin(x);
f1 := x -> cos(x);           # df/dx
x0 := 1.0:                   # sample point
f1exact := f1(x0);           # the exact result for df/dx at x=1.0
lprint(‘f1exact =‘,f1exact): # print value to screen
lprint(‘ ‘):                 # print a blank line
h:= 0.5;                     # initial value of h
n := 15:                     # number of interations
for i from 1 to n do
   Deltaf := f(x0 + h) - f(x0):
   f1approx := Deltaf/h;
   error := f1exact - f1approx;
   lprint(i,‘h =‘,h,‘f1approx =‘,f1approx,‘error =‘,error):
   h := h/10;
od:
```

The output of this program is

```
f1exact =   .5403023059

1   h = .5               f1approx = .3120480036   error = .2282543023
2   h = .5000000000e-1   f1approx = .5190448160   error = .212574899e-1
3   h = .5000000000e-2   f1approx = .5381963800   error = .21059259e-2
4   h = .5000000000e-3   f1approx = .5400920000   error = .2103059e-3
```

```
5    h = .5000000000e-4    f1approx = .5402820000   error = .203059e-4
6    h = .5000000000e-5    f1approx = .5403000000   error = .23059e-5
7    h = .5000000000e-6    f1approx = .5404000000   error = -.976941e-4
8    h = .5000000000e-7    f1approx = .5400000000   error = .3023059e-3
9    h = .5000000000e-8    f1approx = .5400000000   error = .3023059e-3
10    h = .5000000000e-9   f1approx = 1.000000000   error = -.4596976941
11    h = .5000000000e-10  f1approx = 0             error = .5403023059
12    h = .5000000000e-11  f1approx = 0             error = .5403023059
13    h = .5000000000e-12  f1approx = 0             error = .5403023059
14    h = .5000000000e-13  f1approx = 0             error = .5403023059
15    h = .5000000000e-14  f1approx = 0             error = .5403023059
```

Notice that our closest estimate does not occur for the smallest value of h: in fact, once h is smaller than $.5 \times 10^{-6}$ our estimates for $f'(1.0)$ get progressively worse. Indeed, even as we approach the optimal value of h we have a problem; for we start losing significant digits at $i = 3$.

The loss of significant digits can be traced to the *subtraction error* that occurs when we try to compute the difference between two floating point numbers of about the same size: e.g.,

$$1.1234567 \times 10^7 - 1.1234566 \times 10^7 = 0.0000001 \times 10^7$$

The complete failure of this algorithm for very small values of h ($i > 10$) has to do with the fact that there is only a discrete set of machine numbers; for once h gets small enough $f(x+h)$ and $f(x)$ will correspond to the same machine number and so their computed difference will be zero.

In summary, we **can not** improve the accuracy of numerical computations of derivatives by simply making h small enough. What we shall try to do instead is to make our computations as accurate as possible for fixed values of h.

In order to improve matters, let's take a closer look at the error inherent in the approximation

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

Recall that the 1^{st} order Taylor formula with Lagrange Remainder

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(\xi_x)h^2$$

is an exact identity for some point $\xi_x \in [x, x+h]$. Solving this equation for $f'(x)$ we obtain

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2}f''(\xi_x)\,h$$

This tells us that the error involved in estimating $f'(x)$ using (1) is of order h. Now as we seen above, making h smaller as a means of improving our accuracy is only effective up to a point (the point where subtraction and floating point errors kick in). We might therefore look for means for estimating $f'(x)$ such that the error term is of higher order in h.

Here's one simple way to do that. Suppose we take the difference of the following two second order Taylor formulae

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(\xi_1)\,h^3 \quad , \quad \xi_1 \in [x, x+h] \tag{2a}$$

$$f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(\xi_2)\,h^3 \quad , \quad \xi_2 \in [x-h, x] \tag{2b}$$

$$\Rightarrow \qquad f(x+h) - f(x-h) = 2f'(x)h + \frac{1}{6}\left(f'''(\xi_1) - f'''(\xi_2)\right)h^3$$
$$\Rightarrow \qquad f'(x) = \frac{f(x+h)-f(x-h)}{2h} + \frac{1}{6}\left(\frac{f'''(\xi_1) - f'''(\xi_2)}{2}\right)h^2$$
$$\Rightarrow \qquad f'(x) = \frac{f(x+h)-f(x-h)}{2h} + \frac{1}{6}f'''(\xi)\,h^2 \quad , \quad \xi \in [x-h, h+h]$$

where in the last step we have applied the Mean Value Theorem for $f'''(x)$ on the interval $[x-h, x+h]$. We thus arrive at an estimate for $f'(x)$ for which the error term is of order h^2.

If we replace the do-loop in the Maple code above with

```
   for i from 1 to n do
   Deltaf := f(x0 + h) - f(x0 -h):
   f1approx := Deltaf/(2*h);
   error := f1exact - f1approx;
   lprint(i,‘h =‘,h,‘f1approx =‘,f1approx,‘error =‘,error):
   h := h/10;
od:
```

we get the following output

```
1   h = .5              f1approx = .5180694480   error = .222328579e-1
2   h = .5000000000e-1   f1approx = .5400772080   error = .2250979e-3
3   h = .5000000000e-2   f1approx = .5403000500   error = .22559e-5
4   h = .5000000000e-3   f1approx = .5403023000   error = .59e-8
5   h = .5000000000e-4   f1approx = .5403030000   error = -.6941e-6
6   h = .5000000000e-5   f1approx = .5403000000   error = .23059e-5
7   h = .5000000000e-6   f1approx = .5403000000   error = .23059e-5
8   h = .5000000000e-7   f1approx = .5400000000   error = .3023059e-3
9   h = .5000000000e-8   f1approx = .5400000000   error = .3023059e-3
10   h = .5000000000e-9  f1approx = .8000000000   error = -.2596976941
11   h = .5000000000e-10 f1approx = 0             error = .5403023059
12   h = .5000000000e-11 f1approx = 0             error = .5403023059
13   h = .5000000000e-12 f1approx = 0             error = .5403023059
14   h = .5000000000e-13 f1approx = 0             error = .5403023059
15   h = .5000000000e-14 f1approx = 0             error = .5403023059
```

Looking at this data, we see that we have the same problem as before with extremely small values of h. However, we **are** able to achieve an absolute error of 0.59×10^{-8} in 4 steps; which is much better than the earlier method (for which the least error was 0.23059×10^{-5} and which took 6 steps to reach.)

1. Richardson Extrapolation

We can do even better though. Let's assume $f(x)$ is a smooth function so that we can write

$$\begin{aligned} f(x+h) &= \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x) h^k = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \cdots \\ f(x-h) &= \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x) (-h)^k = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(x)h^3 + \cdots \end{aligned}$$

Note that since the series expansions are infinite, we can regard these as exact equations. Subtracting these two equations and solving for $f'(x)$ yields

$$f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] - \left[\frac{1}{3!}f'''(x)h^2 + \frac{1}{5!}f^{(5)}(x)h^4 + \frac{1}{7!}f^{(7)}(x)h^6 + \cdots\right]$$

Let us write this as

$$f'(x) = \phi_0(h) + a_2h^2 + a_4h^4 + a_6h^6 + \cdots \tag{3}$$

where

$$\begin{aligned} \phi_0(h) &= \frac{1}{2h}\left[f(x+h) - f(x-h)\right] \\ a_2 &= \frac{1}{3!}f'''(x) \\ a_4 &= \frac{1}{5!}f^{(5)}(x) \\ a_6 &= \frac{1}{7!}f^{(7)}(x) \\ &\ \vdots \end{aligned}$$

This equation should be true for all small h, in particular for $h/2$. So we should also have

$$f'(x) = \phi_0\left(\frac{h}{2}\right) + a_2\left(\frac{h}{2}\right)^2 + a_4\left(\frac{h}{2}\right)^4 + a_6\left(\frac{h}{2}\right)^6 + \cdots \tag{4a}$$

$$f'(x) = \phi_0\left(\frac{h}{2}\right) + \frac{1}{4}a_2h^2 + \frac{1}{16}a_4h^4 + \frac{1}{64}a_6h^6 \tag{4b}$$

If we then subtract 1/3 times equation (3) from 4/3 times equation (4b) we can arrange it so that the terms of order h^2 cancel, obtaining

$$\begin{aligned} \frac{4}{3}f'(x) &= \frac{4}{3}\phi_0\left(\frac{h}{2}\right) + \frac{1}{3}a_2h^2 + \frac{1}{12}a_4h^4 + \frac{1}{72}a_6h^6 \\ -\frac{1}{3}f'(x) &= -\frac{1}{3}\phi_0(h) - \frac{1}{3}a_2h^2 - \frac{1}{3}a_4h^4 - \frac{1}{3}a_6h^6 + \cdots \end{aligned}$$

$$\begin{aligned} f'(x) &= \left(\frac{4}{3} - \frac{1}{3}\right)f'(x) = -\frac{1}{3}\phi_0(h) + \frac{4}{3}\phi_0\left(\frac{h}{2}\right) - \frac{1}{4}a_4h^4 - \frac{5}{16}a_6h^6 + \cdots \qquad (5) \\ &= -\frac{1}{6h}\left(f(x+h) - f(x-h)\right) + \frac{2}{3h}\left(f(x+h/2) - f(x-h/2)\right) + \mathcal{O}\left(h^4\right) \end{aligned}$$

We thus achieve an expression for $f'(x)$ where the error term is of order h^4.

Having achieved this success, we might as well continue. Equation (5) is good for all sufficiently small h (and in fact, it is exact if the terms indicated by the ... are included). Setting

$$\begin{aligned}\phi_1(h) &= -\frac{1}{3}\phi_0(h) + \frac{4}{3}\phi_0\left(\frac{h}{2}\right) \\ b_4 &= -\frac{1}{4}a_4 \\ b_6 &= -\frac{5}{16}a_6\end{aligned}$$

we can again write down two equivalent expresssions for $f'(x)$

$$\begin{aligned}f^{'}(x) &= \phi_1(h) + b_4 h^4 + b_6 h^6 + \cdots \\ f'(x) &= \phi_1(h/2) + \frac{1}{16}b_4 h^4 + \frac{1}{64}b_6 h^6 +\end{aligned}$$

If we then take subtract $\frac{1}{15}$ times the first equation from $\frac{16}{15}$ times the first we obtain

$$f'(x) = -\frac{1}{15}\phi_1(h) + \frac{16}{15}\phi_1\left(\frac{h}{2}\right) + \frac{1}{15}\left(\frac{1}{4} - 1\right) b_6 h^6$$

We thus obtain an expression for $f'(x)$

$$f'(x) \approx \phi_2(x) \equiv -\frac{1}{15}\phi_1(h) + \frac{16}{15}\phi_1\left(\frac{h}{2}\right)$$

that is accurate to to order h^6. It should be clear that this process can be continued indefinitely in principle, and in practice at least until we exhaust our stamina.

Let's now turn this into a numerical algorithm. The first thing to do is to identify the pattern that mediates the successive expressions for $f'(x)$. We have

$$\begin{aligned}\phi_0(h) &\equiv \frac{f(x+h) - f(x-h)}{2h} \\ \phi_1(h) &= -\frac{1}{3}\phi_0(h) + \frac{4}{3}\phi_0\left(\frac{h}{2}\right) = -\frac{1}{4^1 - 1}\phi_0(h) + \frac{4^1}{4^1 - 1}\phi_0\left(\frac{h}{2}\right) \\ \phi_2(h) &= -\frac{1}{15}\phi_1(h) + \frac{16}{15}\phi_1\left(\frac{h}{2}\right) = -\frac{1}{4^2 - 1}\phi_1(h) + \frac{4^2}{4^2 - 1}\phi_1\left(\frac{h}{2}\right)\end{aligned}$$

and so it would seem

$$\phi_i(h) = -\frac{1}{4^i - 1}\phi_{i-1}(h) + \frac{4^i}{4^i - 1}\phi_{i-1}\left(\frac{h}{2}\right)$$

This is, in fact correct (In fact, it is not too hard to prove this formula using mathematical induction).

Before translating this into computer code. Let's make the following definition. Let

$$R_h[n, i] := \phi_i\left(\frac{h}{2^n}\right)$$

We then have

$$R_h[n, 0] \equiv \phi_0\left(\frac{h}{2^n}\right) = \frac{f\left(x + h/2^n\right) + f\left(x - h/2^n\right)}{h/2^n}$$

and the recursive formulae

$$R_h[n, i] \equiv -\frac{1}{4^i - 1}R_h[n, i-1] + \frac{4^i}{4^i - 1}R_h[n+1, i-1]$$

This quantity $R_h[n, i]$ will be the i^{th} order Richardson Expolation of $f'(x)$ with $h = 2^{-n}$.

The following program calculates the fourth order Richardson Extrapolation of $f'(1.0)$ for $f(x) = \sin(x)$.

```
R[0] := (f(x+h) - f(x-h))/(2*h);
for i from 1 to 4 do
 p1 := R[i-1]/(4^i -1);
 p2 := (4^i)*subs({h=h/2},p1);
 R[i] := p2 - p1;
od:

R4 := R[4];
f := x -> evalf(sin(x));
dfapprox := (x1,h1) -> subs({x=x1,h=h1},R4);

x0 := 1.0;
h0 := 0.1;
for i from 1 to 10 do
 dfR4 := evalf(dfapprox(x0,h0));
 lprint(`h =`,h0,`dfR4 =`, dfR4);
 h0 := h0/10;
od:
```

This program produces the following output.

```
h =   .1               dfR4 =   .5403023038
h =   .1000000000e-1   dfR4 =   .5403023410
h =   .1000000000e-2   dfR4 =   .5403028570
h =   .1000000000e-3   dfR4 =   .5403029364
h =   .1000000000e-4   dfR4 =   .5402236374
h =   .1000000000e-5   dfR4 =   .5418266476
h =   .1000000000e-6   dfR4 =   .506746747
h =   .1000000000e-7   dfR4 =   .71775075
h =   .1000000000e-8   dfR4 =   2.9495862
h =   .1000000000e-9   dfR4 =   0
```

Of course, exact answer is $cos(1.0) = 0.5403023059$. The important thing to note is that we can achive a very accurate result (correct to 7 decimal places) using the very crudest value of h ($h = 0.1$). The fact that we don't get much better results for smaller values of h is again tracable due to the fact that the real source of the problem - the substraction errors inherent to floating point computations, do not miraculously disappear. In fact, one should be aware that in Richardson Extrapolation, subtraction errors tend to kick in much earlier (when one tries to improve accuracy by simplying making h smaller). For example, in computing the fourth order Richardon Extrapolation the computer needs to calculate

$$f\left(x+\frac{h}{2^4}\right) - f\left(x-\frac{h}{2^4}\right)$$

And so in practice, when one employs an n^{th} order Richardson Extrapolation one has to be sure that the n is not too big so that the difference between $f\left(x+h/2^n\right)$ and $f\left(x-h/2^n\right)$ isn't too small to be resolved by the computer.

Let me summarize here closed formulae for the low order Richardson Extrapolations:

Order 0 :

$$\begin{aligned}\frac{df}{dx}(x) &= \phi_0(h) + \mathcal{O}\left(h^2\right)\\ &= \frac{1}{2h}\left(f(x+h) - f(x-h)\right) + \mathcal{O}\left(h^2\right)\end{aligned}$$

Order 1 :

$$\begin{aligned}\frac{df}{dx}(x) &= \phi_1(h) + \mathcal{O}\left(h^4\right)\\ &= -\frac{1}{3}\phi_0(h) + \frac{4}{3}\phi_0\left(\frac{h}{2}\right) + \mathcal{O}\left(h^4\right)\\ &= -\frac{1}{6h}\left(f(x+h) - f(x-h)\right) + \frac{4}{3h}\left(f\left(x+\frac{h}{2}\right) - f\left(x-\frac{h}{2}\right)\right) + \mathcal{O}\left(h^4\right)\end{aligned}$$

Order 2 :

$$\begin{aligned}\frac{df}{dx}(x) &= \phi_2(h) + \mathcal{O}\left(h^6\right)\\ &= -\frac{1}{15}\phi_1(h) + \frac{16}{15}\phi_1\left(\frac{h}{2}\right) + \mathcal{O}\left(h^6\right)\\ &= \frac{1}{90h}\left(f(x+h) - f(x-h)\right) - \frac{4}{9h}\left(f\left(x+\frac{h}{2}\right) = f\left(x-\frac{h}{2}\right)\right) + \frac{128}{45h}\left(f\left(x+\frac{h}{4}\right) - f\left(x-\frac{h}{4}\right)\right) + \mathcal{O}\left(h^6\right)\end{aligned}$$