Numerical Differentiation

We assume that we can compute a function f, but that we have no information about how to compute f'. We want ways of estimating $f'(x)$, given what we know about f.

Reminder: definition of differentiation:

$$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

For second derivatives, we have the definition:

$$\frac{d^2f}{dx^2} = \lim_{\Delta x \to 0} \frac{f'(x+\Delta x) - f'(x)}{\Delta x}$$

First Derivative

We can use this formula, by taking Δx equal to some small value h, to get the following approximation,

- known as the Forward Difference ($D_+(h)$):

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

- Alternatively we could use the interval on the other side of x, to get the Backward Difference ($D_-(h)$) :

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

- A more symmetric form, the Central Difference ($D_0(h)$), uses intervals on either side of x:

$$f'(x) \approx D_0(h) = \frac{f(x+h) - f(x-h)}{2h}$$

All of these give (different) approximations to $f'(x)$.

Second Derivative

The simplest way is to get a symmetrical equation about x by using both the forward and backward differences to estimate $f'(x+\Delta x)$ and $f'(x)$ respectively:

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

Error Estimation in Differentiation I

We shall see that the error involved in using these differences is a form of truncation error (R_T):

$$\begin{aligned} R_T &= D_+(h) - f'(x) \\ &= \tfrac{1}{h}(f(x+h) - f(x)) - f'(x) \end{aligned}$$

Using Taylor's Theorem: $f(x+h) = f(x) + f'(x)h + f''(x)h^2/2! + f^{(3)}(x)h^3/3! + \cdots$:

$$\begin{aligned} R_T &= \tfrac{1}{h}(f'(x)h + f''(x)h^2/2! + f'''(x)h^3/3! + \cdots) - f'(x) \\ &= \tfrac{1}{h}f'(x)h + \tfrac{1}{h}(f''(x)h^2/2! + f'''(x)h^3/3! + \cdots)) - f'(x) \\ &= f''(x)h/2! + f'''(x)h^2/3! + \cdots \end{aligned}$$

Using the Mean Value Theorem, for some ξ within h of x:

$$R_T = \frac{f''(\xi) \cdot h}{2}$$

Error Estimation in Differentiation II

We don't know the value of either f'' or ξ, but we can say that the error is order h:

$$R_T \text{ for } D_+(h) \text{ is } O(h)$$

so the error is proportional to the step size — as one might naively expect.
For $D_-(h)$ we get a similar result for the truncation error — also $O(h)$.

Exercise: differentiation I

Limit of the Difference Quotient. Consider the function $f(x) = e^x$.

1. compute $f'(1)$ using the sequence of approximation for the derivative:

$$D_k = \frac{f(x+h_k) - f(x)}{h_k}$$

with $h_k = 10^{-k}, \quad k \geq 1$

2. for which value k do you have the best precision (knowing $e^1 = 2.71828182845905$). Why?

Exercise: differentiation II

1. `xls/Lect13.xls`
2. Best precision at $k = 8$. When h_k is too small, $f(1)$ and $f(1+h_k)$ are very close together. The difference $f(1+h_k) - f(1)$ can exhibit the problem of loss of significance due to the substraction of quantities that are nearly equal.

Central Difference

- we have looked at approximating $f'(x)$ with the backward $D_-(h)$ and forward difference $D_+(h)$.
- Now we just check out the approximation with the central difference:

$$f'(x) \simeq D_0(h) = \frac{f(x+h) - f(x-h)}{2h}$$

- Richardson extrapolation

Error analysis of Central Difference I

We consider the error in the Central Difference estimate ($D_0(h)$) of $f'(x)$:

$$D_0(h) = \frac{f(x+h) - f(x-h)}{2h}$$

We apply Taylor's Theorem,

$$\begin{array}{rcl}
f(x+h) & = & f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \cdots \quad (A) \\
f(x-h) & = & f(x) - f'(x)h + \frac{f''(x)h^2}{2!} - \frac{f'''(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \cdots \quad (B) \\
(A)-(B) & = & 2f'(x)h + 2\frac{f'''(x)h^3}{3!} + 2\frac{f^{(5)}(x)h^5}{5!} + \cdots \\
\frac{(A)-(B)}{2h} & = & f'(x) + \frac{f'''(x)h^2}{3!} + \frac{f^{(5)}(x)h^4}{5!} + \cdots
\end{array}$$

Error analysis of Central Difference II

We see that the difference can be written as

$$D_0(h) = f'(x) + \frac{f''(x)}{6}h^2 + \frac{f^{(4)}(x)}{24} + \cdots$$

or alternatively, as

$$D_0(h) = f'(x) + b_1 h^2 + b_2 h^4 + \cdots$$

where be know how to compute b_1, b_2, etc.

We see that the error $R_T = D_0(h) - f'(x)$ is $O(h^2)$.

Remark. Remember: for D_- and D_+, the error is $O(h)$.

Error analysis of Central Difference III

Example.
Let try again the example:

$$f(x) = e^x \qquad f'(x) = e^x$$

We evaluate $f'(1) = e^1 \approx 2.71828...$ with

$$D_0(h) = \frac{f(1+h) - f(1-h)}{2h}$$

for $h = 10^{-k}, \quad k \geq 1$.
Numerical values: `xls/Lect13.xls`

Rounding Error in Difference Equations I

- When presenting the iterative techniques for root-finding, we ignored rounding errors, and paid no attention to the potential error problems with performing subtraction. This did not matter for such techniques because:
  1. the techniques are *self-correcting*, and tend to cancel out the accumulation of rounding errors
  2. the iterative equation $x_{n+1} = x_n - c_n$ where c_n is some form of *correction* factor has a subtraction which is safe because we are subtracting a small quantity (c_n) from a large one (e.g. for Newton-Raphson, $c_n = \frac{f(x)}{f'(x)}$).

Rounding Error in Difference Equations II

- However, when using a difference equation like

$$D_0(h) = \frac{f(x+h) - f(x-h)}{2h}$$

we seek a situation where h is small compared to everything else, in order to get a good approximation to the derivative. This means that $x+h$ and $x-h$ are very similar in magnitude, and this means that for most f (well-behaved) that $f(x+h)$ will be very close to $f(x-h)$. So we have the worst possible case for subtraction: the difference between two large quantities whose values are very similar.

- We cannot *re-arrange* the equation to get rid of the subtraction, as this difference is inherent in what it means to compute an approximation to a derivative (differentiation uses the concept of difference in a deeply intrinsic way).

Rounding Error in Difference Equations III

- We see now that the total error in using $D_0(h)$ to estimate $f'(x)$ has two components
  1. the truncation error R_T which we have already calculated,
  2. and a function calculation error R_{XF} which we now examine.
- When calculating $D_0(h)$, we are not using totally accurate computations of f, but instead we actually compute an approximation $\bar{f}$, to get

$$\bar{D}_0(h) = \frac{\bar{f}(x+h) - \bar{f}(x-h)}{2h}$$

- We shall assume that the error in computing f near to x is bounded in magnitude by ϵ:

$$|\bar{f}(x) - f(x)| \leq \epsilon$$

Rounding Error in Difference Equations IV

- The calculation error is then given as

$$\begin{aligned}
R_{XF} &= \bar{D}_0(h) - D_0(h) \\
&= \frac{\bar{f}(x+h) - \bar{f}(x-h)}{2h} - \frac{f(x+h) - f(x-h)}{2h} \\
&= \frac{\bar{f}(x+h) - \bar{f}(x-h) - (f(x+h) - f(x-h))}{2h} \\
&= \frac{\bar{f}(x+h) - f(x+h) - (\bar{f}(x-h) - f(x-h))}{2h} \\
|R_{XF}| &\leq \frac{|\bar{f}(x+h) - f(x+h)| + |\bar{f}(x-h) - f(x-h)|}{2h} \\
&\leq \frac{\epsilon + \epsilon}{2h} \\
&\leq \frac{\epsilon}{h}
\end{aligned}$$

So we see that R_{XF} is proportional to $1/h$, so as h shrinks, this error grows, unlike R_T which shrinks quadratically as h does.

Rounding Error in Difference Equations V

- We see that the total error R is bounded by $|R_T| + |R_{XF}|$, which expands out to

$$|R| \leq \left|\frac{f'''(\xi)}{6}h^2\right| + \left|\frac{\epsilon}{h}\right|$$

So we see that to minimise the overall error we need to find the value of $h = h_{opt}$ which minimises the following expression:

$$\frac{f'''(\xi)}{6}h^2 + \frac{\epsilon}{h}$$

Unfortunately, we do not know f''' or ξ !
Many techniques exist to get a good estimate of h_{opt}, most of which estimate f''' numerically somehow. These are complex and not discussed here.

Richardson Extrapolation I

- The trick is to compute $D_0(h)$ for 2 different values of h, and combine the results in some appropriate manner, as guided by our knowledge of the error behaviour.

In this case we have already established that

$$D_0(h) = \frac{f(x+h) - f(x-h)}{2h} = f'(x) + b_1 h^2 + O(h^4)$$

We now consider using twice the value of h:

$$D_0(2h) = \frac{f(x+2h) - f(x-2h)}{4h} = f'(x) + b_1 4h^2 + O(h^4)$$

We can subtract these to get:

$$D_0(2h) - D_0(h) = 3b_1 h^2 + O(h^4)$$

We divide across by 3 to get:

$$\frac{D_0(2h) - D_0(h)}{3} = b_1 h^2 + O(h^4)$$

Richardson Extrapolation II

The righthand side of this equation is simply $D_0(h) - f'(x)$, so we can substitute to get

$$\frac{D_0(2h) - D_0(h)}{3} = D_0(h) - f'(x) + O(h^4)$$

This re-arranges (carefully) to obtain

$$\begin{aligned}
f'(x) &= D_0(h) + \tfrac{D_0(h) - D_0(2h)}{3} + O(h^4) \\
&= \tfrac{4D_0(h) - D_0(2h)}{3} + O(h^4)
\end{aligned}$$

Richardson Extrapolation III

- It is an estimate for $f'(x)$ whose truncation error is $O(h^4)$, and so is an improvement over D_0 used alone.
- This technique of using calculations with different h values to get a better estimate is known as **Richardson Extrapolation**.

Richardson's Extrapolation.
Suppose that we have the two approximations $D_0(h)$ and $D_0(2h)$ for $f'(x)$, then an improved approximation has the form:

$$f'(x) = \frac{4D_0(h) - D_0(2h)}{3} + O(h^4)$$

Summary

- Approximation for numerical differentiation:

Approximation for $f'(x)$	Error
Forward/backward difference D_+, D_-	$O(h)$
Central difference D_0	$O(h^2)$
Richardson Extrapolation	$O(h^4)$

- Considering the total error (approximation error + calculation error):

$$|R| \le \left|\frac{f'''(\xi)}{6}h^2\right| + \left|\frac{\epsilon}{h}\right|$$

remember that h should not be chosen too small.

Solving Differential Equations Numerically

Definition.
The Initial value Problem deals with finding the solution $y(x)$ of

$$y' = f(x, y) \quad \text{with the initial condition} \quad y(x_0) = y_0$$

- It is a 1st order differential equations (D.E.s).
- Alternative ways of writing $y' = f(x, y)$ are:

$$\begin{aligned} y'(x) &= f(x, y) \\ \frac{dy(x)}{dx} &= f(x, y) \end{aligned}$$

Working Example

- We shall take the following D.E. as an example:

$$f(x, y) = y$$

or $y' = y$ (or $y'(x) = y(x)$).

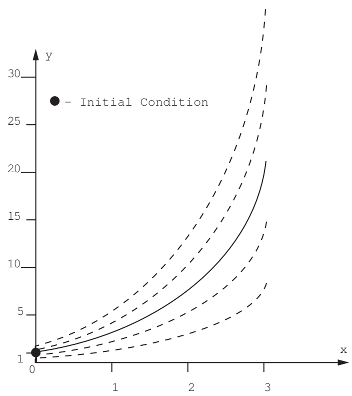
- This has an infinite number of solutions:

$$y(x) = C \cdot e^x \qquad \forall C \in \mathbb{R}$$

- We can single out one solution by supplying an initial condition $y(x_0) = y_0$.
- So, in our example, if we say that $y(0) = 1$, then we find that $C = 1$ and out solution is

$$y = e^x$$

Working Example



The dashed lines show the many solutions for different values of C. The solid line shows the solution singled out by the initial condition that $y(0) = 1$.

The Lipschitz Condition I

We can give a condition that determines when the initial condition is sufficient to ensure a unique solution, known as the Lipschitz Condition.

Lipschitz Condition:
For $a \le x \le b$, for all $-\infty < y, y^* < \infty$, if there is an L such that

$$|f(x, y) - f(x, y^*)| \le L\,|y - y^*|$$

Then the solution to $y' = f(x, y)$ is unique, given an initial condition.

- L is often referred to as the Lipschitz Constant.
- A useful estimate for L is to take $\left|\frac{\partial f}{\partial y}\right| \le L$, for x in (a, b).

The Lipschitz Condition II

Example.
given our example of $y' = y = f(x,y)$, then we can see do we get a suitable L.

$$\begin{aligned}\frac{\partial f}{\partial y} &= \frac{\partial(y)}{\partial(y)} \\ &= 1\end{aligned}$$

So we shall try $L = 1$

$$\begin{aligned}|f(x,y) - f(x,y^*)| &= |y - y^*| \\ &\leq 1 \cdot |y - y^*|\end{aligned}$$

So we see that we satisfy the Lipschitz Condition with a Constant $L = 1$.

Numerically solving $y' = f(x,y)$

- We assume we are trying to find values of y for x ranging over the interval $[a,b]$.
- We start with the one point where we have the exact answer, namely the initial condition $y_0 = y(x_0)$.
- We generate a series of x-points from $a = x_0$ to b, separated by a small step-interval h:

$$x_0 = a$$
$$\left|\begin{aligned} x_i &= a + i \cdot h \\ h &= \tfrac{b-a}{N}\end{aligned}\right.$$
$$x_N = b$$

- we want to compute $\{y_i\}$, the approximations to $\{y(x_i)\}$, the true values.

Euler's Method

- The technique works by using applying f at the current point (x_n, y_n) to get an estimate of y' at that point.

Euler's Method.
This is then used to compute y_{n+1} as follows:

$$y_{n+1} = y_n + h \cdot f(x_n, y_n)$$

This technique for solving D.E.'s is known as Euler's Method.

- It is simple, slow and inaccurate, with experimentation showing that the error is $O(h)$.

Euler's Method

Example.
In our example, we have

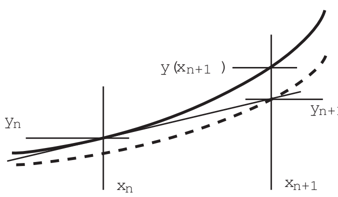
$$y' = y \qquad f(x,y) = y \qquad y_{n+1} = y_n + h \cdot y_n$$

At each point after x_0, we accumulate an error, because we are using the slope at x_n to estimate y_{n+1}, which assumes that the slope doesn't change over interval $[x_n, x_{n+1}]$.

Truncation Errors I

Definitions.

- The error introduced at each step is called the Local Truncation Error.
- The error introduced at any given point, as a result of accumulating all the local truncation errors up to that point, is called the Global Truncation Error.



In the diagram above, the local truncation error is $y(x_{n+1}) - y_{n+1}$.

Truncation Errors II

We can estimate the local truncation error $y(x_{n+1}) - y_{n+1}$, by assuming the value y_n for x_n is exact as follows: as follows:

$$y(x_{n+1}) = y(x_n + h)$$

Using Taylor Expansion about $x = x_n$

$$y(x_{n+1}) = y(x_n) + hy'(x_n) + \frac{h^2}{2} y''(\xi)$$

Assuming y_n is exact ($y_n = y(x_n)$), so $y'(x_n) = f(x_n, y_n)$

$$y(x_{n+1}) = y_n + hf(x_n, y_n) + \frac{h^2}{2} y''(\xi)$$

Now looking at y_{n+1} by definition of the Euler method:

$$y_{n+1} = y_n + hf(x_n, y_n)$$

We subtract the two results:

$$y(x_{n+1}) - y_{n+1} = -\frac{h^2}{2} y''(\xi)$$

Truncation Errors III

So

$$y(x_{n+1}) - y_{n+1} \propto O(h^2)$$

- We saw that the local truncation error for Euler's Method is $O(h^2)$.
- By integration (accumulation of error when starting from x_0), we see that global error is $O(h)$.

As a general principle, we find that if the Local Truncation Error is $O(h^{p+1})$, then the Global Truncation Error is $O(h^p)$.

Introduction

Considering the problem of solving differential equations with one initial condition, we learnt about:

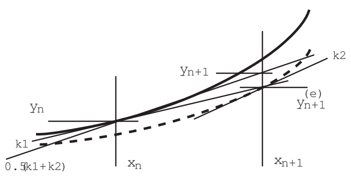
- Lipschitz Condition (unicity of the solution)
- finding numerically the solution : Euler method

Today is about how to improve the Euler's algorithm:

- Heun's method
- and more generally Runge-Kutta's techniques.

Improved Differentiation Techniques I

We can improve on Euler's technique to get better estimates for y_{n+1}. The idea is to use the equation $y' = f(x, y)$ to estimate the slope at x_{n+1} as well, and then average these two slopes to get a better result.



Improved Differentiation Techniques II

- Using the slope $y'(x_n, y_n) = f(x_n, y_n)$ at x_n, the Euler approximation is:

$$(A) \qquad \frac{y_{n+1} - y_n}{h} \simeq f(x_n, y_n)$$

- Considering the slope $y'(x_{n+1}, y_{n+1}) = f(x_{n+1}, y_{n+1})$ at x_{n+1} , we can propose this new approximation:

$$(B) \qquad \frac{y_{n+1} - y_n}{h} \simeq f(x_{n+1}, y_{n+1})$$

- The trouble is: we dont know y_{n+1} in f (because this is what we are looking for!).
- So instead we use $y_{n+1}^{(e)}$, the Euler's approximation of y_{n+1}:

$$(B) \qquad \frac{y_{n+1} - y_n}{h} \simeq f(x_{n+1}, y_{n+1}^{(e)})$$

Improved Differentiation Techniques III

So considering the two approximations of $\frac{y_{n+1} - y_n}{h}$ with expressions (A) and (B), we get a better approximation by averaging (ie. by computing A+B/2):

$$\frac{y_{n+1} - y_n}{h} \simeq \frac{1}{2} \cdot \left(f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(e)} \right)$$

Heun's Method.

The approximation:

$$\begin{aligned} y_{n+1} &= y_n + \tfrac{h}{2} \cdot \left(f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(e)} \right) \\ &= y_n + \tfrac{h}{2} \cdot \left(f(x_n, y_n) + f(x_{n+1}, y_n + h \cdot f(x_n, y_n)) \right) \end{aligned}$$

is known as Heun's Method.

It can be shown to have a global truncation error that is $O(h^2)$. The cost of this improvement in error behaviour is that we evaluate f twice on each h-step.

Runge-Kutta Techniques I

- We can repeat the Heun's approach by considering the approximations of slopes in the interval $[x_n; x_{n+1}]$.
- This leads to a large class of improved differentiation techniques which evaluate f many times at each h-step, in order to get better error performance.
- This class of techniques is referred to collectively as Runge-Kutta techniques, of which Heun's Method is the simplest example.
- The classical Runge-Kutta technique evaluates f four times to get a method with global truncation error of $O(h^4)$.

Runge-Kutta Techniques II

Runge-Kutta's technique using 4 approximations.

It is computed using approximations of the slope at x_n, x_{n+1} and also two approximations at mid interval $x_n + \frac{h}{2}$:

$$\frac{y_{n+1} - y_n}{h} = \frac{1}{6}\left(f_1 + 2 \cdot f_2 + 2 \cdot f_3 + f_4\right)$$

with

$$f_1 = f\left(x_n, y_n\right)$$

$$f_2 = f\left(x_n + \tfrac{h}{2}, y_n + \tfrac{h}{2} f_1\right)$$

$$f_3 = f\left(x_n + \tfrac{h}{2}, y_n + \tfrac{h}{2} f_2\right)$$

$$f_4 = f\left(x_{n+1}, y_n + h \cdot f_3\right)$$

It can be shown that the global truncation error is $O(h^4)$.