Lecture 13

Last time we did Richardson Extrapolation.

This consists of using two lower order approximation's to create a higher order approximation.

$$M = N(h) + K_1 h + K_2 h^2 + K_3 h^3 + K_4 h^4 + \cdots$$

h suff small

$$M = N(h/2) + K_1 \frac{h}{2} + K_2 h^2/4 + K_3 h^3/8 + \cdots$$

One can eliminate $K_1 h$ to get $O(h^2)$ formula

We then studied Romberg integration. This is Richardson extrapolation applied to composite trapezoidal rule.

$$I = \int_a^b f(x)\,dx = T_N + C_2 h^2 + C_4 h^4 + C_6 h^6 + C_8 h^8 + \cdots$$

One eliminates $C_2 h^2$ to get $O(h^4)$ approximation and so forth.

Numerical Differentiation

$f(x)$

we need to compute $f'(x)$

Done when $f(x)$ is not known analytically.

Only a table of function values is known

This is usually the case in

boundary valued diff. eqn's.

example

x	$f(x)$	app $f'(x)$	Exact
0.2	0.1987	0.9680	0.9801
0.3	0.2955	0.9390	0.9553
0.4	0.3894	0.9000	0.9211
0.5	0.4794	0.9000	0.8776

we know $f'(a) = \lim_{h \to 0} \dfrac{f(a+h) - f(a)}{h}$

So one can think of $\frac{f(a+h)-f(a)}{h}$ to be approximation of f

Note we can also take h to be $-$ve.

Above example $f(x) = \sin x$

Thus the above formula has a lot of error

So we compute other formulas to compute $f'(a)$.

We also need "error estimates".

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basic idea

$$f(x) \approx P_k(x)$$

$P_k(x)$ interpolates $f(x)$ at $x_0, \ldots, x_n$

$$f'(x) \approx P_k'(x)$$

$f : [a,b] \to \mathbb{R}$ continuously diff

$x_0, x_1, \ldots, x_k$ distinct pts in $[a,b]$

$$f(x) = P_k(x) + f[x_0, x_1, \ldots, x_k, x]\, \psi_k(x)$$

where $P_k(x)$ interpolates f at $x_0, x_1, \ldots, x_k$

$$\psi_k(x) = \prod_{i=0}^{k} (x - x_i)$$

$$f'(x) = P_k'(x) + \left(\frac{d}{dx} f[x_0, \ldots x_k, x]\right) \psi_k(x)$$

$$+ f[x_0, x_1, \ldots, x_k, x]\, \psi_k'(x)$$

$$\frac{d}{dx} f[x_0, x_1, \ldots, x_k, x] = f[x_0, x_1, \ldots, x_k, x, x]$$

$$f'(x) = P_k'(x) + \underline{f[x_0, \ldots, x_k, x, x]\, \psi_k(x)}$$

$$+ \underline{f[x_0, \ldots x_k]\, \psi_k'(x)}$$

We approximate $f'(a)$ by $P_k'(a)$

So error $= f[x_0, \ldots x_k, a, a]\, \psi_k(a)$

$$+ f[x_0, \ldots x_k, a]\, \psi_k'(a)$$

So $$E(f) = \frac{f^{(k+2)}(\xi)}{(k+2)!}\, \psi_k(a) + \frac{f^{(k+1)}(\eta)}{(k+1)!}\, \psi_k'(a)$$

for some $\xi, \eta \in (c, d)$

This expression tells us very little about the true error, since in practice we usually do not know $f^{(k+1)}$ & $f^{(k+2)}$ involved in $E(f)$ and we will almost never know ξ, η.

So we try to find situations where the error term can be simplified.

Case 1

a is one of the interpolation pts

$a = x_i$ for some i

Since $\psi_k(x)$ contains factor $(x - x_i)$

we get $\psi_k(a) = 0$. So first term

in error drops out.

Moreover $\psi_k'(a) = q(a)$ where

$$q(x) = \frac{\psi_k(x)}{x - x_i} = \prod_{\substack{j=0 \\ j \neq i}}^{k} (x - x_j)$$

Thus $$E(f) = \frac{f^{(k+1)}(\eta)}{(k+1)!} \cdot \prod_{\substack{j=0 \\ j \neq i}}^{k} (x_i - x_j)$$

Case 2

We choose a such that $\psi_k'(a) = 0$

So the second term in error formula vanishes

k is odd then we can achieve this by placing x_i's symmetrically around a; so that

$$(*) \quad x_{k-j} - a = a - x_j \qquad j = 0, 1, \dots, \frac{k-1}{2}$$

Then

$$(x - x_j)(x - x_{k-j}) = (x-a)^2 - (a - x_j)^2$$

$$j = 0, 1, \dots, \frac{k-1}{2}$$

$$\psi_k(x) = \prod_{j=0}^{\frac{k-1}{2}} \left[(x-a)^2 - (a-x_j)^2 \right]$$

Since $\frac{d}{dx}\left[(x-a)^2 - (a-x_j)^2 \right]\Big|_{x=a} = 0$

We get $\psi_k'(a) = 0$.

Thus if (*) holds then error formula reduces to

$$E(f) = \frac{1}{(k+2)!} f^{(k+2)}(\xi) \prod_{j=0}^{\frac{k-1}{2}} \left[-(a-x_j)^2\right]$$

Specific examples

$k=1$

$$P_k(x) = f(x_0) + f[x_0, x_1](x - x_0)$$

$$D(P_k) = f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

Case 1 $a = x_0$ and $h = x_1 - x_0$

we get

$$f'(a) \approx f[a, a+h] = \frac{f(a+h) - f(a)}{h}$$

$$E(f) = -\frac{1}{2} h f''(\eta)$$

Case 2 $\quad a = \frac{x_0 + x_1}{2}$.

x_0, x_1 are symmetric w.r.t a

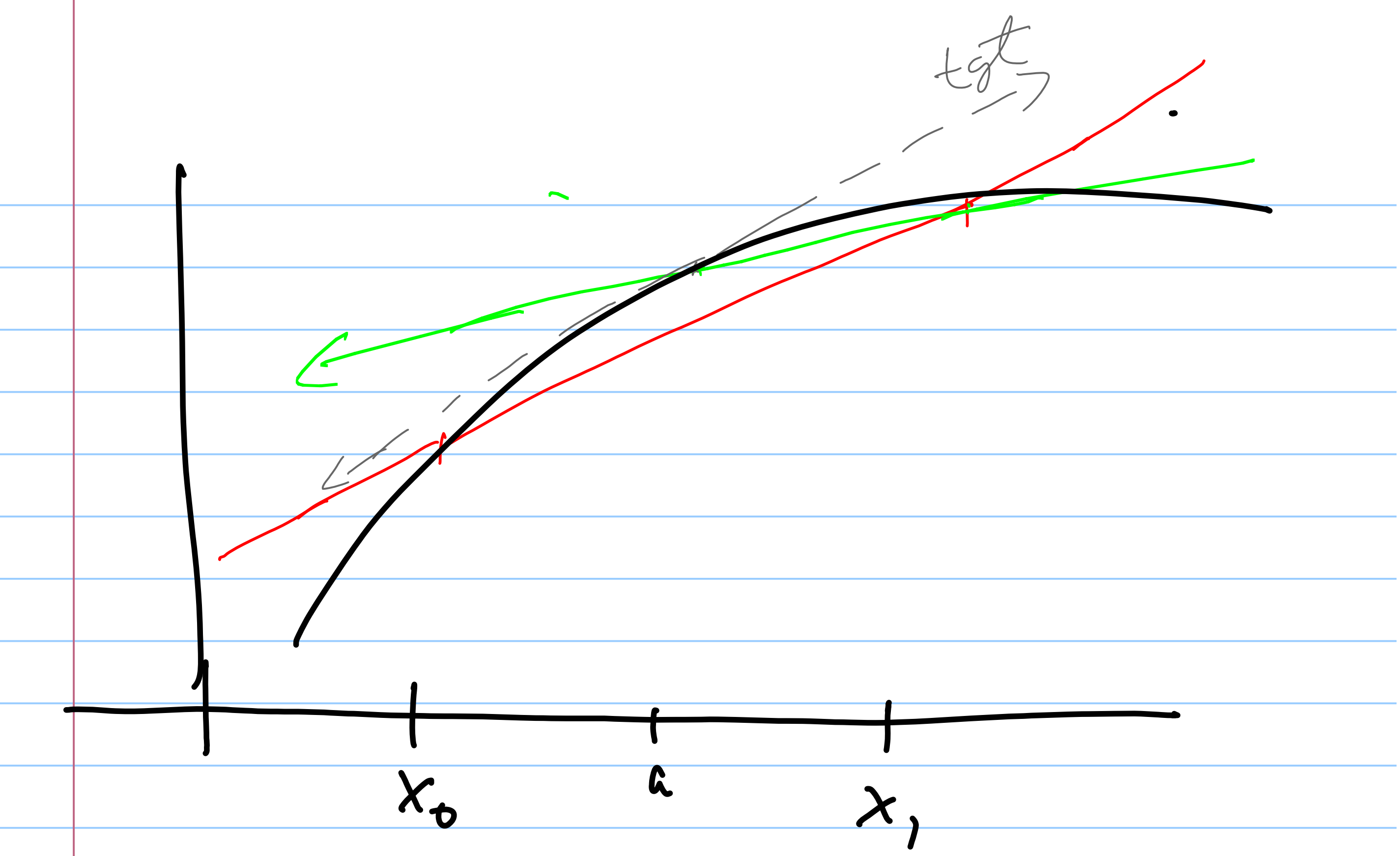
$x_0 = a - h, \quad x_1 = a + h, \quad h = \frac{1}{2}(x_1 - x_0)$

We get central-difference formula

$$f'(a) \approx f[a-h, a+h] = \frac{f(a+h) - f(a-h)}{2h}$$

$$E(f) = -\frac{h^2}{6} f'''(\xi)$$

Here if x_0, x_1 are close together then $f[x_0, x_1]$ is a much better approx to $f'(a)$ at the midpt $a = \frac{1}{2}(x_0 + x_1)$ than at the either end pt $a = x_0$ or $a = x_1$



Next we consider using three interpolation pts so that $k=2$

$$P_k(x) = f[x_0] + f[x_0, x_1](x - x_1) + f[x_0, x_1, x_2](x - x_1)(x - x_2)$$

$$P_k'(x) = f[x_0, x_1] + f[x_0, x_1, x_2](2x - x_1 - x_2)$$

So if $a = x_0$ then we get

$$f'(a) \approx f[a, x_1] + f[a, x_1, x_2](a - x_1)$$

$$E(f) = \frac{1}{6}(a - x_1)(a - x_2) f'''(\eta)$$

In particular $x_1 = a + h$, $x_2 = a + 2h$

$$f'(a) \approx \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h}$$

$$E(f) = \frac{h^2}{3} f'''(\xi)$$ for some ξ between a, $a+2h$

Example

x	$f(x)$	computed $f'(x)$	exact
0.2	0.1987	0.9825	0.9801
0.3	0.2955	0.9535	0.9553
0.4	0.3894	0.9195	0.9211
0.5	0.4794	0.8805	0.8776

One can also get higher derivatives of f

$$f''(x) \approx p_k''(x)$$

$k=2, \quad a = x_0 \qquad x_1 = a+h \qquad x_2 = a+2$

$$f''(a) \approx \frac{f(a) - 2f(a+h) + f(a+2h)}{h^2}$$

$$E(f) = \frac{h^2}{6} f^{(iv)}(\xi) - h f'''(\eta)$$

$a = x_0 \qquad x_1 = a-h, \quad x_2 = a+h$

we see

$$f''(a) \approx \frac{f(a-h) - 2f(a) + f(a+h)}{h^2}$$

$$E(f) = -\frac{h^2}{12} f^{(iv)}(\xi)$$

Thus placing interpolation points symmetrically around a has resulted in a higher order formula

Numerical diff is a "bad" problem

i.e., by getting h smaller it is prone to lot of round off error

(since we are subtracting nearly same quantities).

Furthermore we are also dividing by a small number

Thus Numerical differentiation has to be done with care.

Ways to improve accuracy

Richardson extrapolation

(1) $$f(a+h) = f(a) + f'(a)h + \frac{f''(a)}{2}h^2 + \frac{f'''(a)}{6}h^3 + \frac{f^{iv}(a)}{24}h^4 + \frac{f^{v}(a)}{120}h^5 + o(h^5)$$

(2) $$f(a-h) = f(a) - f'(a)h + \frac{f''(a)}{2}h^2 - \frac{f'''(a)}{6}h^3 + \frac{f^{iv}(a)}{24}h^4 - \frac{f^{v}(a)}{120}h^5 + o(h^5)$$

$\frac{(1) - (2)}{2h}$ gives

$$\frac{f(a+h) - f(a-h)}{2h} = f'(a) + \frac{f'''(a)}{6}h^2 + \frac{f^{(v)}(a)}{120}h^4 + o(h^5)$$

Thus $f'(a) = D(h) + c_2 h^2 + c_4 h^4 + \cdots$

$$D(h) = \frac{f(a+h) - f(a-h)}{2h}$$