ERG 2012B

Advanced Engineering Mathematics II

Part III

Introduction to Numerical Methods

Lectures #19

Difference Formulas,

Numerical Integrations & Differentiation

Newton's Forward Difference Formula

The previous formula is valid for *arbitrarily spaced* nodes which might occur in practice in experiments. However in many applications the x_j are ***regular spaced***. Then we can write:

$$x_0, \quad x_1 = x_0 + h, \quad x_2 = x_0 + 2h, \cdots, \quad x_n = x_0 + nh$$

We define the ***k*th forward difference** of f at x_j recursively by

$$\Delta^k f_j = \Delta^{k-1} f_{j+1} - \Delta^{k-1} f_j \qquad (k = 1,2,.....)$$

with the **first forward difference** defined as:

$$\Delta f_j = f_{j+1} - f_j$$

It can then be shown by induction (see text book) that

$$f[x_0, \cdots, x_k] = \frac{1}{k!h^k} \Delta^k f_0$$

It clearly works for $k = 1$ as $x_1 = x_0 + h$ so that

$$f[x_0, x_1] = \frac{f_1 - f_0}{x_1 - x_0} = \frac{1}{1!h} \Delta f_0$$

Newton's Forward Difference Formula

Setting $x=x_0+rh$ in the divided difference formula so that $x-x_0=rh$, $x-x_1=(r-1)h$ etc.. we obtain **Newton's forward difference interpolation formula**

$$f(x) \approx p_n(x) = \sum_{s=0}^{n} \binom{r}{s} \Delta^s f_0 \qquad (r = (x - x_0)/h)$$

$$= f_0 + r\Delta f_0 + \frac{r(r-1)}{2!}\Delta^2 f_0 + \cdots + \frac{r(r-1)\cdots(r-n+1)}{n!}\Delta^n f_0$$

where the **binomial coefficients** are defined by

$$\binom{r}{0} = 1, \quad \binom{r}{\mathrm{s}} = \frac{r(r-1)\cdots(r-s+1)}{s!} \quad (s > 0, \text{integer})$$

Newton's Forward Difference Formula

Errors. As before

$$\varepsilon_n(x) = f(x) - p_n(x) = (x - x_0)(x - x_1)\cdots(x - x_n)\frac{f^{(n+1)}(t)}{(n+1)!}$$

and $x - x_0 = rh$, $x - x_1 = (r - 1)\,h$ etc.. so that:

$$\varepsilon_n(x) = \frac{h^{n+1}}{(n+1)!} r(r-1)\cdots(r-n) f^{(n+1)}(t)$$

Note:

(1) ε_n is about the order of magnitude of the next difference not used in $p_n(x)$

(2) Choose $x_0,\ldots,x_n$ such that the x at the interpolation is as well centered between $x_0,\ldots x_n$ as possible

Example 5

Compute cosh(0.56) from the given values

		Difference Table			
j	x_j	$f_j = f(x_j)$	Δf_j	$\Delta^2 f_j$	$\Delta^3 f_j$
0	0.5	1.127626			
			0.057839		
1	0.6	1.185465		0.011865	
			0.069704		0.000698
2	0.7	1.255169		0.012562	
			0.082266		
3	0.8	1.337435			

given values (rows j = 0 to 3)

we use the shaded numbers in the polynomial and
r=(0.56-0.50)/0.1 = 0.6

$$f(x) \approx f_0 + r\Delta f_0 + \frac{r(r-1)}{2}\Delta^2 f_0 + \frac{r(r-1)(r-2)}{6}\Delta^3 f_0$$

$$\cosh(0.56) \approx 1.127626 + 0.6 \cdot 0.057839 + \frac{0.6(-0.4)}{2} 0.011865 + \frac{0.6(-0.4)(-1.4)}{6} 0.000698$$

$$= 1.160944$$

Example 5

Error Estimate: since $\cosh^{(4)}t = \cosh t$

$$\text{and} \quad \varepsilon_n(x) = \frac{h^{n+1}}{(n+1)!} r(r-1)\cdots(r-n) f^{(n+1)}(t)$$

$$\varepsilon_3(x) = \frac{h^4}{(4)!} r(r-1)\cdots(r-3)\cosh(t)$$

now $r = 0.6, \quad x = 0.56$ and $h = 0.1$ then

$$\varepsilon_3(0.56) = \frac{0.1^4}{(4)!} 0.6(-0.4)(-1.4)(-2.4)\cosh(t)$$

$$= -0.00000336 \cosh t$$

where $0.5 \le t \le 0.8$

Since $f(x)=p_3(x)+\varepsilon_3(x)$ we have

$p_3(0.56)+0.00000336 \cosh(0.8) \le \cosh(0.56) \le p_3(0.56)+0.00000336 \cosh(0.5)$

Numerically:

$$1.160939 \le \cosh(0.56) \le 1.160941$$

Newton's Backward Difference Formula

Without changing the difference table we can make a harmless change to the running subscript *j* and create the **backward difference formula** for equally spaced x_j

$$x_0,\quad x_1 = x_0 + h,\quad x_2 = x_0 + 2h, \cdots,\quad x_n = x_0 + nh$$

We define the ***k*^th^ backward difference** of *f* at x_j recursively by

$$\nabla^k f_j = \nabla^{k-1} f_j - \nabla^{k-1} f_{j-1} \quad (k = 1, 2, \ldots.)$$

with the **first backward difference** defined as:

$$\nabla f_j = f_j - f_{j-1}$$

And **Newton's backward difference interpolation formula:**

$$f(x) \approx p_n(x) = \sum_{s=0}^{n} \binom{r+s-1}{s} \nabla^s f_0 \qquad (r = (x - x_0)/h)$$

$$= f_0 + r\nabla f_0 + \frac{r(r+1)}{2!}\nabla^2 f_0 + \cdots + \frac{r(r+1)\cdots(r+n-1)}{n!}\nabla^n f_0$$

Central Difference Notation

There is a third notation for difference, the **central difference notation**

We define the ***k*^th^ central difference** of f at x_j recursively by

$$\delta^k f_j = \delta^{k-1} f_{j+\frac{1}{2}} - \delta^{k-1} f_{j-\frac{1}{2}} \qquad (j = 2,3,....)$$

with the **first central difference** defined as:

$$\delta f_j = f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}$$

So that in this notation a difference table e.g. for f_{-1}, f_0, f_1, f_2 looks as follows:

x_{-1}	f_{-1}			
		$\delta f_{-½}$		
x_0	f_0		$\delta^2 f_0$	
		$\delta f_{½}$		$\delta^3 f_{½}$
x_1	f_1		$\delta^2 f_1$	
		$\delta f_{1+½}$		
x_2	f_2			

Example 6

Compute a 7D value of the Bessel function $J_0(x)$ for x=1.72 from the values given

given values (rows j for = 0 to 3)

			Difference Table			
j for	***j bk***	***x j***	***J 0(x j)***	**1st Diff**	**2nd Diff**	**3rd Diff**
0	-3	1.7	0.3979849			
				-0.0579985		
1	-2	1.8	0.3399864		-0.0001693	
				-0.0581678		0.0004093
2	-1	1.9	0.2818186		0.0002400	
				-0.0579278		
3	0	2.0	0.2238908			

we use the yellow shaded numbers in the *forward* polynomial and the pink ones in the *backward* polynomial so that:

$$r = \frac{(1.72 - 1.70)}{0.1} = 0.2$$

$$J_0(1.72) \approx 0.3979849 + 0.2(-0.0579985) + \frac{0.2(-0.8)}{2}(-0.0001693) + \frac{0.2(-0.8)(-1.8)}{6}0.0004093 = 0.3864183$$

Example 6

Compute a 7D value of the Bessel function $J_0(x)$ for x=1.72 from the values given

given values

			Difference Table			
j for	*j bk*	*x j*	*J 0(x j)*	1st Diff	2nd Diff	3rd Diff
0	-3	1.7	0.3979849			
				-0.0579985		
1	-2	1.8	0.3399864		-0.0001693	
				-0.0581678		0.0004093
2	-1	1.9	0.2818186		0.0002400	
				-0.0579278		
3	0	2.0	0.2238908			

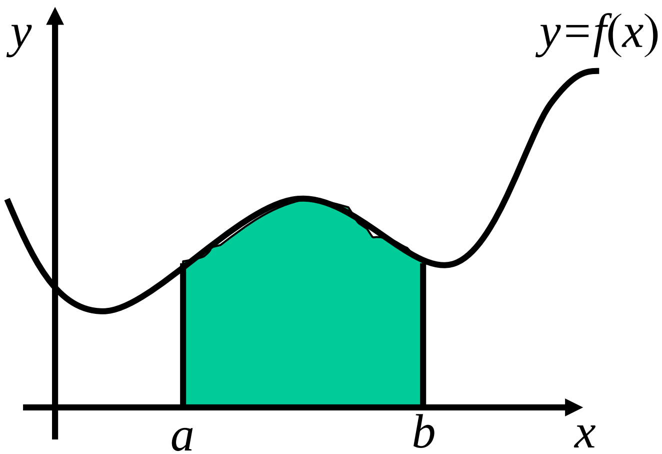
we use the yellow shaded numbers in the *forward* polynomial and the pink ones in the *backward* polynomial so that:

$$r = \frac{(1.72 - 2.00)}{0.1} = 2.8$$

$$J_0(1.72) \approx 0.2238908 - 2.8(-0.0579278) + \frac{-2.8(-1.8)}{2} 0.0002400 + \frac{-2.8(-1.8)(-0.8)}{6} 0.0004093 = 0.3864184$$

Numerical Integration

$$J = \int_a^b f(x)dx$$



where *a* and *b* are given and *f* is a function given analytically by a formula or empirically by a table of values.

•geometrically, *J* is the area *under* the curve of *f* between *a* and *b*

Numerical integration methods are obtained by approximating the integrand *f* by functions that can easily be integrated.

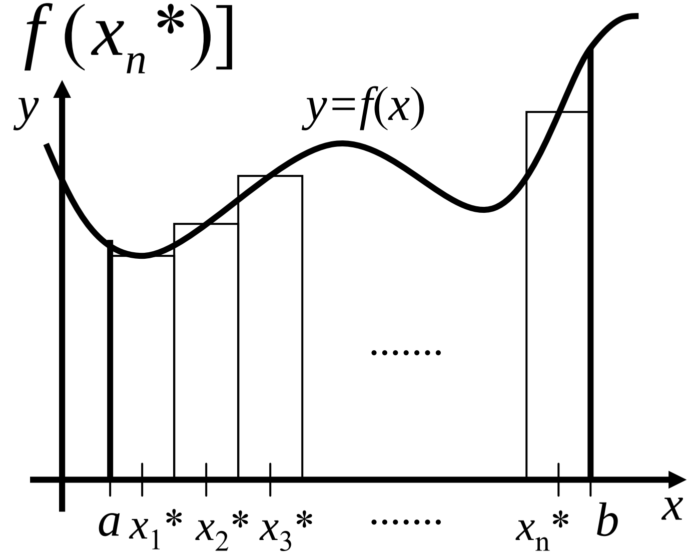
Rectangular Rule

The simplest formula, **the rectangular rule**, is obtained if we:

- subdivide the interval of integration into n subintervals of equal length $h=(b-a)/n$
- in each subinterval approximate each f by the constant $f(x_j^*)$, the value of f at the midpoint x_j^* of the j^{th} subinterval
- f is then approximated by a set of n rectangles of areas $f(x_1^*)h,\ldots,f(x_n^*)h$ giving the rectangular rule:

$$J = \int_a^b f(x)dx \approx h[f(x_1^*) + f(x_2^*) + \cdots + f(x_n^*)]$$

where $h=(b-a)/n$



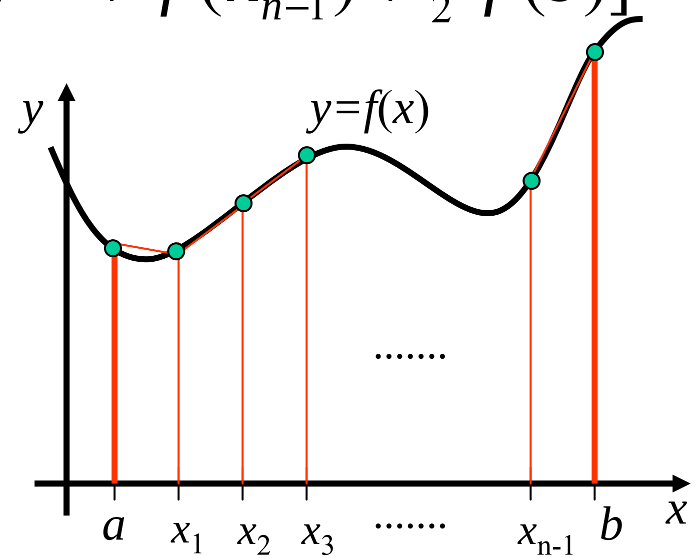
Trapezoidal Rule

The **trapezoidal rule**, is generally more accurate:

- subdivide in the same way
- approximate *f* by a broken line of segments with end points $[a, f(a)]$, $[x_1, f(x_1)]$,...$[b, f(b)]$ on the curve of *f*
- *f* is then approximated by a set of *n* trapezoids of areas $\frac{1}{2}[f(a)+f(x_1)]h$,..., $\frac{1}{2}[f(x_{n-1})+f(b)]h$ giving the trapezoidal rule:

$$J = \int_a^b f(x)dx \approx h[\tfrac{1}{2} f(a) + f(x_1) + f(x_2) \cdots + f(x_{n-1}) + \tfrac{1}{2} f(b)]$$

where $h=(b-a)/n$



Error bounds for the Trapezoidal Rule

The error estimate can be made in a similar way as before

$$\varepsilon_n(x) = f(x) - p_n(x) = (x - x_0)(x - x_1)\cdots(x - x_n)\frac{f^{(n+1)}(t)}{(n+1)!}$$

with n=1, beginning with a single subinterval:

$$\varepsilon_1(x) = f(x) - p_1(x) = (x - x_0)(x - x_1)\frac{f''(t)}{2}$$

with a suitable t (between x_0 and x_1)

Integration over x from x_0 to x_0+h gives:

$$\int_{x_0}^{x_0+h} f(x)dx - \frac{h}{2}[f(x_0) + f(x_1)] = \int_{x_0}^{x_0+h} (x - x_0)(x - x_0 - h)\frac{f''(t)}{2}dx$$

Error bounds for the Trapezoidal Rule

setting $x\text{-}x_0=v$ the right hand side becomes:

$$\int_0^h v(v-h)dv\,\frac{f''(\tilde{t})}{2}=\left(\frac{h^3}{3}-\frac{h^3}{2}\right)\frac{f''(\tilde{t})}{2}=-\frac{h^3}{12}f''(\tilde{t})$$

where $\tilde{t}$ is a suitable value between x_0 and x_1 Hence the overall error is the sum of n such contributions from n subintervals and since $h=(b\text{-}a)/n$ we obtain:

$$\varepsilon=-\frac{(\mathrm{b-a})^3}{12n^2}f''(\hat{t})$$

with $\hat{t}$ between a and b

Error Bounds are obtained by taking the largest f'', M_2 and the smallest, M_2* over the interval of integration, so that:

$$KM_2\le\varepsilon\le KM_2{}^*\quad\text{where}\quad K=-\frac{(\mathrm{b-a})^3}{12n^2}$$

Example 1

Evaluate $J = \int_0^1 e^{-x^2} dx$ by trapezoidal rule with $n = 10$

Computational Table

j	*xj*	*xj2*	exp(-*x* j2)	
0	0.0	0.00	1.000000	
1	0.1	0.01		0.990050
2	0.2	0.04		0.960789
3	0.3	0.09		0.913931
4	0.4	0.16		0.852144
5	0.5	0.25		0.778801
6	0.6	0.36		0.697676
7	0.7	0.49		0.612626
8	0.8	0.64		0.527292
9	0.9	0.81		0.444858
10	1.0	1.00	0.367879	
Sums			1.367879	6.778168

$$J = \int_a^b f(x)dx \approx h[\tfrac{1}{2} f(a) + f(x_1) + f(x_2) \cdots + f(x_{n-1}) + \tfrac{1}{2} f(b)]$$

Therefore: $J \approx 0.1(0.5 \cdot 1.367879 + 6.778168) = 0.746212$

Example 2

Estimate the error in Example 1.

Solution: From

$$KM_2 \le \varepsilon \le KM_2^* \quad \text{where} \quad K = -\frac{(b-a)^3}{12n^2}$$

where M_2 and M_2^* are the largest and smallest values of $f^{//}(x)$ in the region of integration

By differentiation $f^{//}(x) = 2(2x^2 - 1)\exp(-x^2)$

Also $f^{///}(x) > 0$ for $0>x>1$ so the minumum and maximum occur at the ends of the interval.

Therefore $M_2 = f^{//}(1)=0.735759$ and $M_2^* = f^{//}(0) = -2$

and K=-1200 so that

$$-0.000614 \le \varepsilon \le 0.001667$$

and exact value of J lies between 0.745597 and 0.747878