

Numerical Differentiation

Finite Difference Differentiation

Formal Definition of the Derivative $f'(x_o) = \lim_{h \rightarrow 0} \frac{f(x_o + h) - f(x_o)}{h}$

If we simply let h be “small”, we have an approximation to the derivative,

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

If $h > 0$ this is a *forward-difference* formula and if $h < 0$ this is a *backward-difference* formula.

It has a unique relation to the Taylor series for $f(x_o + h)$

$$f(x_o + h) = f(x_o) + hf'(x_o) + \frac{1}{2}h^2 f''(\xi), \quad \xi \in (x_o, x_o + h)$$

$$f'(x_o) = \frac{f(x_o + h) - f(x_o)}{h} + \frac{h}{2} f''(\xi)$$

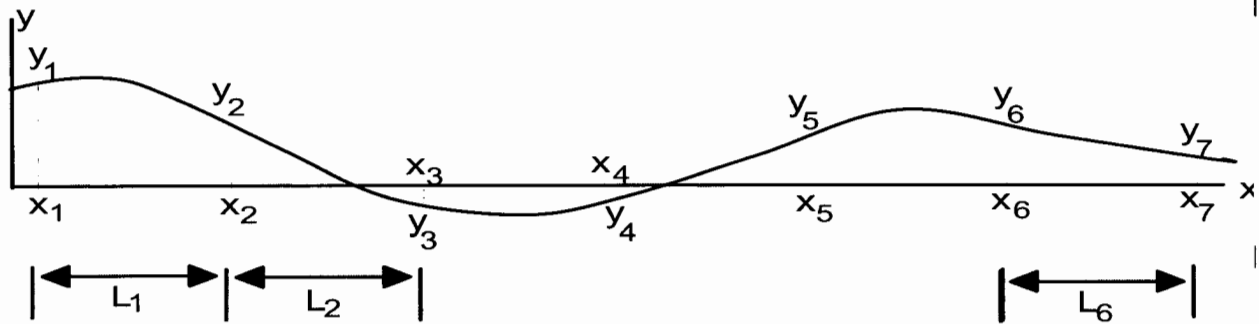
Our approximation to the derivative is obtained by dropping the last term which introduces an error of $O(h)$. The smaller the value of h , the smaller the mathematical error. However, very small h results in numerical subtraction of two “nearly identical” numbers so it introduces round-off error.

A *centered difference* formula for the derivative is:

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

The error in this formula is $O(h^2)$

Sometimes the points are not equally spaced so numerical implementation of the centered difference formula is impossible. Consider the case of $y = f(x)$ with values at specific points known as sketched below:



For all interior points (x_2 to x_6) in the figure, interpolation of derivatives at the center of adjacent points can be used to generate the equivalent of a centered difference formula at each of the x-points, even when the distances, L , are not equal.

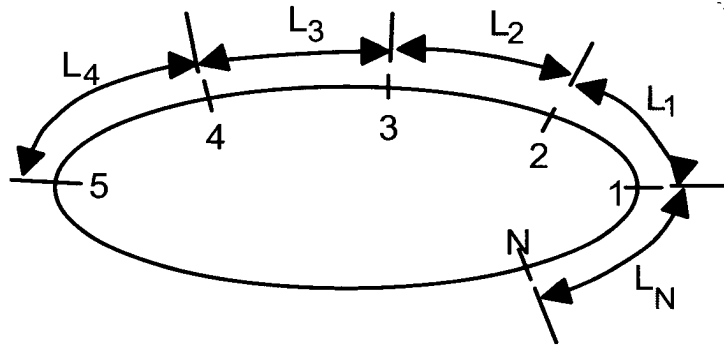
The resulting formula is:

$$f'(x_m) = y_m \frac{q_m - q_{m-1}}{2 q_m q_{m-1}} + \frac{1}{2} \left[\frac{y_{m+1}}{q_m} - \frac{y_{m-1}}{q_{m-1}} \right] \tag{1}$$

$$\text{where: } q_m = \frac{1}{2}(L_{m+1} + L_m)$$

For estimating the derivatives at the end points, extrapolation can be used from the numerical derivative half way between the two endmost points using the forward or backward difference formula and the the derivative at the nearest interior point given by the above formula.

Sometimes values of a function, y , are given at unequally spaced points around the periphery of a plane curve as sketched below.



The lengths L are arc lengths (s) between points on the curve and values of y are known at points (1, 2, ..., N) on the curve. To obtain the numerical approximation of the tangential derivative $y'(s)$ at points 1,2,3, N , equation (1) can be used. However, for point $m = 1$, special values for some of the y 's and some of the L 's must be used. In particular $y_{m-1} = y_N$ and $L_{m-1} = L_N$.

Likewise for for point $m = N$, $y_{m+1} = y_1$ and $L_{m+1} = L_1$.

To estimate the error in Simpson's rule, the function over four successive points can be expanded in a Taylor series up to order 3. With equally spaced points, the error in the integral from the cubic term vanishes and the dominant term in the error is proportional to the fourth derivative $d^4 f/dx^4$. For equally spaced points with $h = \Delta x$, the total error, E_T takes the form:

$$E_T = -\frac{h^5}{90} \sum_{i=1}^{n-1} \frac{d^4 f(\eta_i)}{dx^4}$$

η_i is some value of x in the i^{th} interval.

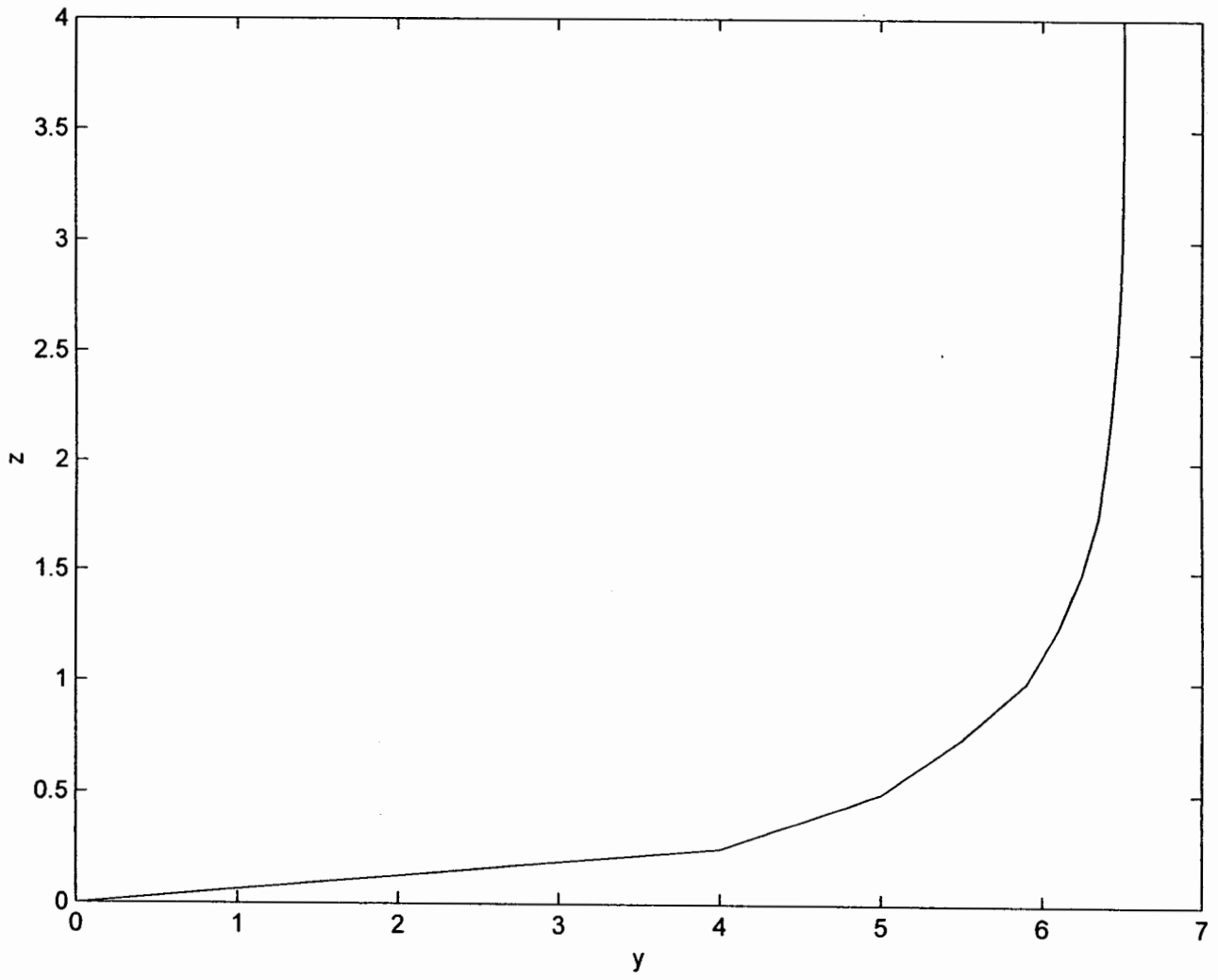
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numint
%SCRIPT TO DO NUMERICAL INTEGRATION WITH EQUALLY SPACED POINTS
fil = input('Enter input file name: ','s');
fid = fopen(fil,'r');
n = fscanf(fid,'%d',1);
for k = 1:n;
    z(k) = fscanf(fid, '%f', 1);
    y(k) = fscanf(fid, '%f', 1);
end;
h = z(2) - z(1);
Ir = 0;
It = 0;
Is = 0;
for k = 2:n-1
    Ir = Ir + y(k);
    It = It + y(k);
end;
Ir = h*(Ir+y(1));
It = h*(It + 0.5*y(1) + 0.5*y(n));
for k = 1:2:n-2;
    Is = Is + y(k) + 4.0*y(k+1) + y(k+2);
end;
Is = Is*h/3.0 ;
fprintf(1, '%s \n', 'Integrals from Rectangular, Trapezoidal and Simpson's Rules');
fprintf(1, '%9.5f %9.5f %9.5f \n', Ir, It, Is);

```

shipsec

| | |
|------|-------|
| 17 | 0.000 |
| 0.00 | 4.000 |
| 0.25 | 5.000 |
| 0.50 | 5.500 |
| 0.75 | 5.900 |
| 1.00 | 6.100 |
| 1.25 | 6.250 |
| 1.50 | 6.350 |
| 1.75 | 6.400 |
| 2.00 | 6.440 |
| 2.25 | 6.470 |
| 2.50 | 6.490 |
| 2.75 | 6.500 |
| 3.00 | 6.504 |
| 3.25 | 6.507 |
| 3.50 | 6.509 |
| 3.75 | 6.510 |
| 4.00 | |



```
>> numint
Enter input file name: shipsec.txt
Integrals from Rectangular, Trapezoidal and Simpson's Rules
22.73000    23.54375    23.67800
>>
```