Richardson extrapolation:

If the composite trapezoidal rule is used to evaluate an integral twice, once using a step size of h_1 and once using a step size of h_2, we have:

$$I = I(h_1) + E(h_1) = I(h_2) + E(h_2)$$

$$\begin{aligned} \text{where } I &= \text{true value of integral} \\ I(h_i) &= \text{value obtained using } h_i \\ E(h_i) &= \text{error when using } h_i \end{aligned}$$

The errors are roughly proportional to the squares of the the step sizes:

$$E(h) \cong -\frac{(b-a)^3}{12n^2}\bar{f}''(\zeta) = -\frac{(b-a)h^2}{12}\bar{f}''(\zeta)$$

$$\therefore \quad \frac{E(h_1)}{E(h_2)} \cong \frac{h_1^{\,2}}{h_2^{\,2}} \qquad\qquad E(h_1) \cong E(h_2)\left(\frac{h_1}{h_2}\right)^2$$

Eliminating $E(h_1)$ from the original equation and solving for $E(h_2)$ gives:

$$I(h_1)+E(h_2)\left(\frac{h_1}{h_2}\right)^2 \cong I(h_2)+E(h_2)$$

$$E(h_2) \cong \frac{I(h_1)-I(h_2)}{1-(h_1/h_2)^2}$$

This result leads to a useful expression for the true value of the integral:

$$I = I(h_2)+E(h_2)$$

$$\cong I(h_2)+\frac{I(h_1)-I(h_2)}{1-(h_1/h_2)^2}$$

The equation takes two estimates with errors of order h^2 and produces an estimate with an error of order h^4.

When $h_2 = h_1/2$ (when the step size is halved) the equation becomes:

$$I \cong \frac{4}{3}I(h_2)-\frac{1}{3}I(h_1)$$

Example:

Suppose we want to evaluate $\int_1^9 xe^{-0.2x}dx$

Solving analytically (or using *integral*) gives I = 12.9910004

Composite trapezoidal integration with h = 8 gives $I(8)$ = 9.2256830 (29% error)

Composite trapezoidal integration with h = 4 gives $I(4)$ = 11.9704303 (7.9% error)

Combining the two estimates gives an improved estimate:

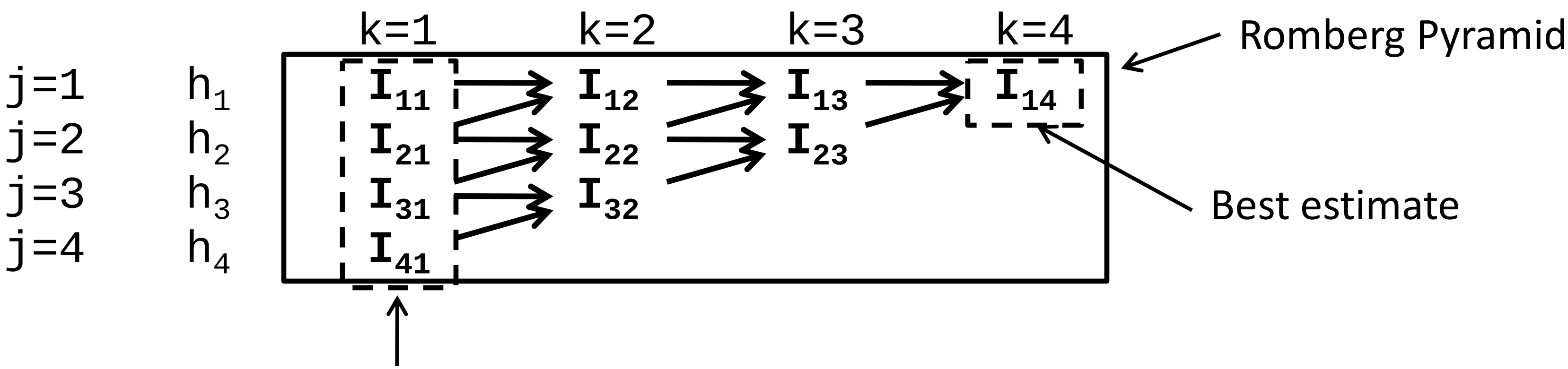
$$I \cong \frac{4}{3}I(4) - \frac{1}{3}I(8) = 12.8853461 \quad \text{(0.8\% error)}$$

The two initial integrations involve a grand total of three function evaluations (the two points used to find $I(8)$ can be reused in finding $I(4)$)

Interesting point: Applying Simpson's 1/3 rule to the three points gives exactly the same result. This will always be the case when $h_1 = b - a$ (try proving this).

Romberg integration:

The improved estimates obtained by combining initial estimates can be combined to produce still better estimates and so on.



Initial estimates (obtained using ever smaller step sizes)

$$I_{j,k} = \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1} \qquad h_j = \frac{h_1}{2^{j-1}}$$

Example (same problem as last slide, analytical result = 12.991000416828392):

```
 9.225682988289043  12.885346094001475  12.990342105576776  12.990999499741445
11.970430317573367  12.983779854853319  12.990989227957623
12.730442470533331  12.990538642138604
12.925514599237287
```

This pyramid required a total of just nine function evaluations.

The relative error in the best estimate can be approximated by using the difference between this estimate and the best estimate at the previous level of refinement

		k=1	k=2	k=3	k=4	
j=1	h_1	$\mathbf{I}_{11}$	$\mathbf{I}_{12}$	$\mathbf{I}_{13}$	$\boxed{\mathbf{I}_{14}}$	Best estimate
j=2	h_2	$\mathbf{I}_{21}$	$\mathbf{I}_{22}$	$\boxed{\mathbf{I}_{23}}$		Best estimate at previous level
j=3	h_3	$\mathbf{I}_{31}$	$\mathbf{I}_{32}$			
j=4	h_4	$\mathbf{I}_{41}$				

Relative error formula: $$|\varepsilon| = \left| \frac{I_{1,k} - I_{2,k-1}}{I_{1,k}} \right| \times 100\%$$

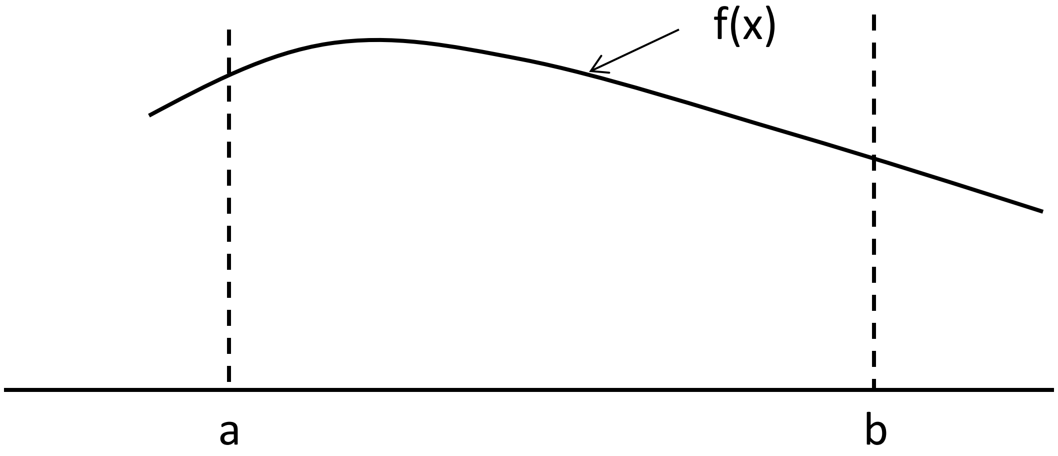
The pyramid size is increased (by adding further initial estimates) until the relative error becomes acceptably small

Added entries

		k=1	k=2	k=3	k=4	k=5
j=1	h_1	$\mathbf{I}_{11}$	$\mathbf{I}_{12}$	$\mathbf{I}_{13}$	$\mathbf{I}_{14}$	$\boxed{\mathbf{I}_{15}}$
j=2	h_2	$\mathbf{I}_{21}$	$\mathbf{I}_{22}$	$\mathbf{I}_{23}$	$\boxed{\mathbf{I}_{24}}$	
j=3	h_3	$\mathbf{I}_{31}$	$\mathbf{I}_{32}$	$\boxed{\mathbf{I}_{33}}$		
j=4	h_4	$\mathbf{I}_{41}$	$\boxed{\mathbf{I}_{42}}$			
j=5	h_5	$\boxed{\mathbf{I}_{51}}$				

Gaussian quadrature:

Suppose that we must estimate the integral of some function over an interval and that we are only allowed to evaluate the function twice (perhaps the function takes a lot of time to evaluate).

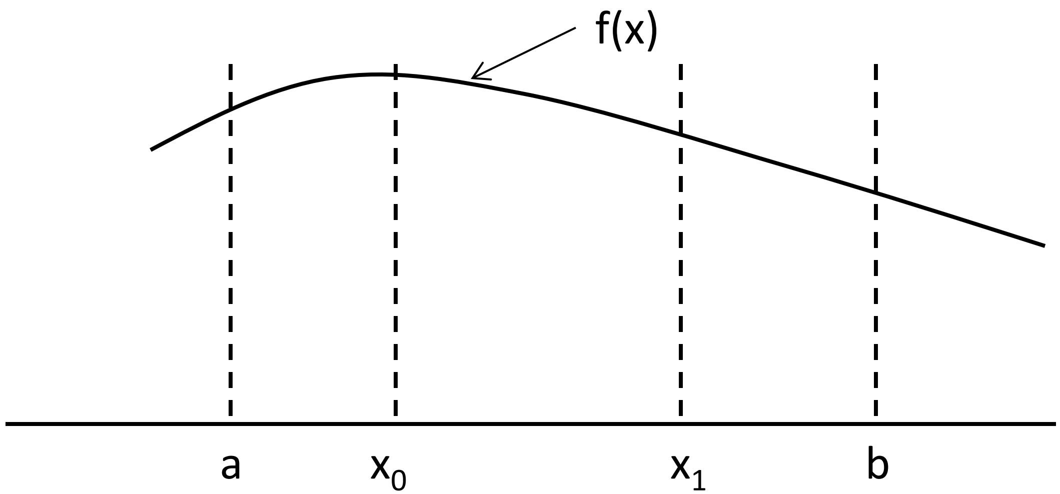


We could evaluate the function at the end points of the interval and use trapezoidal integration:

$$I = (b-a)\frac{f(a)+f(b)}{2}$$

But is this the best approach?

Suppose that a better answer can be obtained by using two points (x_0 and x_1) within the interval

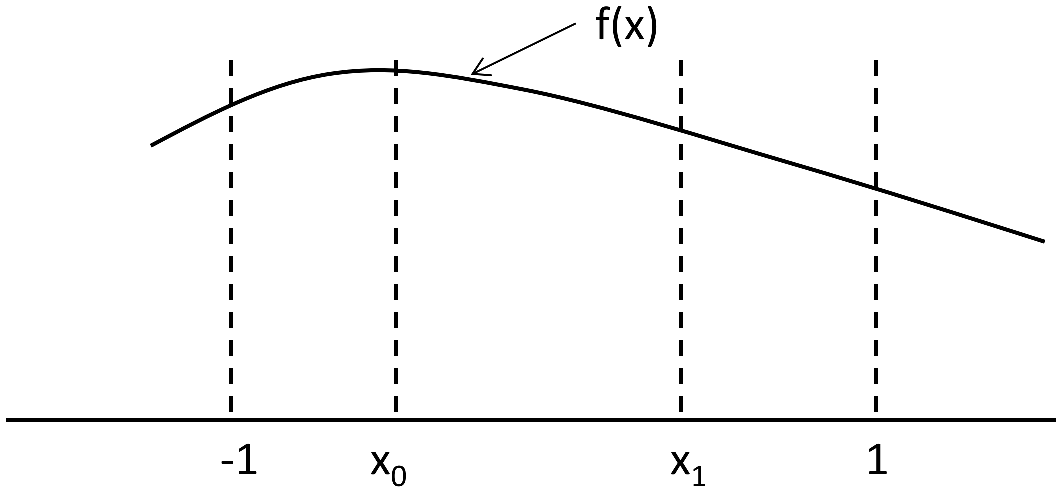


The integral will be estimated by applying two coefficients (c_0 and c_1) to the values of the function at the two points

$$I = c_0 f(x_0) + c_1 f(x_1)$$

We need to find the values for x_0, x_1, c_0 and c_1
Solving for these four unknowns requires four equations.

To simplify the analysis, it is assumed that that a = -1 and b = 1



Requiring that the integral be exact if $f(x) = k$ gives

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} f(x)dx$$

$$c_0 k + c_1 k = \int_{-1}^{1} k dx$$

$$c_0 + c_1 = 2$$

Requiring that the integral be exact if $f(x) = kx$ gives

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} f(x)dx$$

$$c_0 k x_0 + c_1 k x_1 = \int_{-1}^{1} kxdx$$

$$c_0 x_0 + c_1 x_1 = 0$$

Requiring that the integral be exact if $f(x) = kx^2$ gives

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} f(x)dx$$

$$c_0 k x_0{}^2 + c_1 k x_1{}^2 = \int_{-1}^{1} kx^2 dx$$

$$c_0 x_0{}^2 + c_1 x_1{}^2 = \frac{2}{3}$$

Requiring that the integral be exact if *f*(*x*) = *kx*³ gives

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} f(x)dx$$

$$c_0 k x_0^{\ 3} + c_1 k x_1^{\ 3} = \int_{-1}^{1} kx^3 dx$$

$$c_0 x_0^{\ 3} + c_1 x_1^{\ 3} = 0$$

Solving the four equations simultaneously gives

$$x_0 = -\frac{1}{\sqrt{3}} = -0.57735\ldots \qquad x_1 = \frac{1}{\sqrt{3}} = -0.57735\ldots$$

$$c_0 = c_1 = 1$$

$$I = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

Example:

$$f(x) = x^3 - 2x^2 + 4x - 3 \qquad \int_{-1}^{1} f(x)\, dx = ????$$

Analytically:

$$I = \left. \frac{x^4}{4} - \frac{2x^3}{3} + \frac{4x^2}{2} - 3x \right|_{-1}^{1} = -7.33333\overline{3}$$

Using Gaussian quadrature:

$$I = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = (-6.168517833) + (-1.1648155) = -7.33333\overline{3}$$

Keep in mind that the magic only works perfectly for polynomials of order <= 3.

If the limits of integration are not -1 and 1 a change of variable is required

$$f(x) = x^3 - 2x^2 + 4x - 3 \qquad \int_1^5 f(x)\,dx = ????$$

Analytically:

$$I = \left|\frac{x^4}{4} - \frac{2x^3}{3} + \frac{4x^2}{2} - 3x\right|_1^5 = 109.33333\overline{3}$$

To change variable:

$$x \Rightarrow \frac{b+a}{2} + \frac{b-a}{2} x_d \qquad dx \Rightarrow \frac{b-a}{2} dx_d$$

$$\int_a^b f(x)\,dx \Rightarrow \int_{-1}^{1} f\left(\frac{b+a}{2} + \frac{b-a}{2} x_d\right)\frac{b-a}{2} dx_d = \int_{-1}^{1} F(x_d)\,dx_d$$

In this case:

$$\int_1^5 f(x)\,dx \Rightarrow = \int_{-1}^{1} f(3+2x_d)(2)dx_d = \int_{-1}^{1} F(x_d)\,dx_d$$

$$F(x_d) = f(3+2x_d)(2) = 2\left((3+2x_d)^3 - 2(3+2x_d)^2 + 4(3+2x_d) - 3\right)$$

$$I = F\left(-\frac{1}{\sqrt{3}}\right) + F\left(\frac{1}{\sqrt{3}}\right) = 7.708845 + 101.62449 = 109.333335$$

The principle can be extended to 3, 4, and more points:

Points:	2	3	4
x0	-0.577350	-0.774597	-0.861136
c0	1	5/9	0.347855
x1	0.577350	0	-0.339981
c1	1	8/9	0.652145
x2		0.774597	0.339981
c2		5/9	0.652145
x3			0.861136
c3			0.347855
Error	$f^{(4)}(\xi)$	$f^{(6)}(\xi)$	$f^{(8)}(\xi)$

With four points the magic works perfectly for polynomials of order <= 7.

Adaptive quadrature:

Used by quad and quadl

Step size for subintervals adjusted until a satisfactory result is obtained

The net effect is that smaller steps are used in areas where the function changes rapidly and larger steps are used in areas where it doesn’t

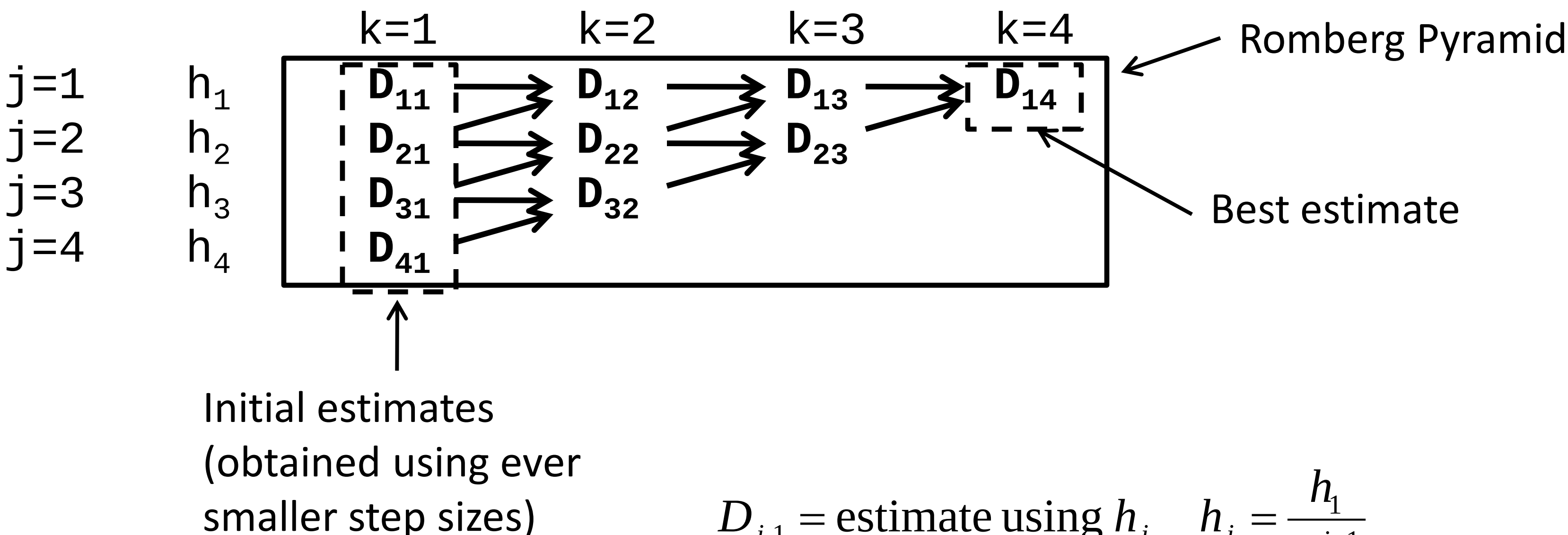
Numerical Differentiation:

First Derivative	"First order"	"Second Order" (better)
Forward	$\frac{f(x_{i+1})-f(x_i)}{h}$	$\frac{-f(x_{i+2})+4f(x_{i+1})-3f(x_i)}{2h}$
Backwards	$\frac{f(x_i)-f(x_{i-1})}{h}$	$\frac{3f(x_i)-4f(x_{i-1})+f(x_{i-2})}{2h}$
Central	$\frac{f(x_{i+1})-f(x_{i-1})}{2h}$	$\frac{-f(x_{i+2})+8f(x_{i+1})-8f(x_{i-1})+f(x_{i-2})}{12h}$

Richardson extrapolation and differentiation:

Richardson extrapolation can be used to refine derivate estimates

The process is entirely analogous to the process for refining integral estimates



$$D_{j,1} = \text{estimate using } h_j \qquad h_j = \frac{h_1}{2^{j-1}}$$

$$D_{j,k} = \frac{4^{k-1} D_{j+1,k-1} - D_{j,k-1}}{4^{k-1} - 1} \qquad |\varepsilon| = \left| \frac{D_{1,k} - D_{2,k-1}}{D_{1,k}} \right|$$

Differentiation and Matlab:

Function *diff*:

Usage: deltas = diff (x)

Accepts a vector of length n and produces a vector of length n – 1

$deltas(i) = x(i + 1) - x(i)$

Function *gradient*:

Usage: xd = gradient(x)

Accepts a vector of length n and produces a vector of length n

For i not equal to 1 or n: $xd(i) = (x(i + 1) - x(i - 1)) / 2$ % centered difference
$xd(1) = x(2) - x(1)$ % forward difference
$xd(n) = x(n) - x(n-1)$ % backward difference

If x values evenly spaced and 1 apart result is the numerical derivative
For other evenly spaced data the result must be divided by the step size

Example: The distance that a skydiver falls in time *t* is given by

$$dist(t) = \frac{m}{c_d} \ln\left[\cosh\left(\left(\sqrt{\frac{gc_d}{m}}\right)t\right)\right]$$

Determine and plot the skydiver's velocity for *t* from 0 to 10 seconds

```
% distance function
dist = @(t) (m / cd) * log (cosh(sqrt(g * cd/m)*t));

h = 2.0;                  % chosen step size
t = 0: h: 10;             % time values
s = dist(t);              % generate corresponding distance values
v = gradient(s) / h;      % perform numeric differentiation

plot (t, v, ‘b');         % plot results
grid on;
```

The plot below shows the actual velocity as well as the velocity obtained by numerical differentiation

Note the significant discrepancy at $t = 0$

Reducing the step size gives progressively better results