Integration and quadrature

Riemann sums and why they are bad

The trapezoidal rule and Simpson’s rule

The adaptive trapezoidal algorithm

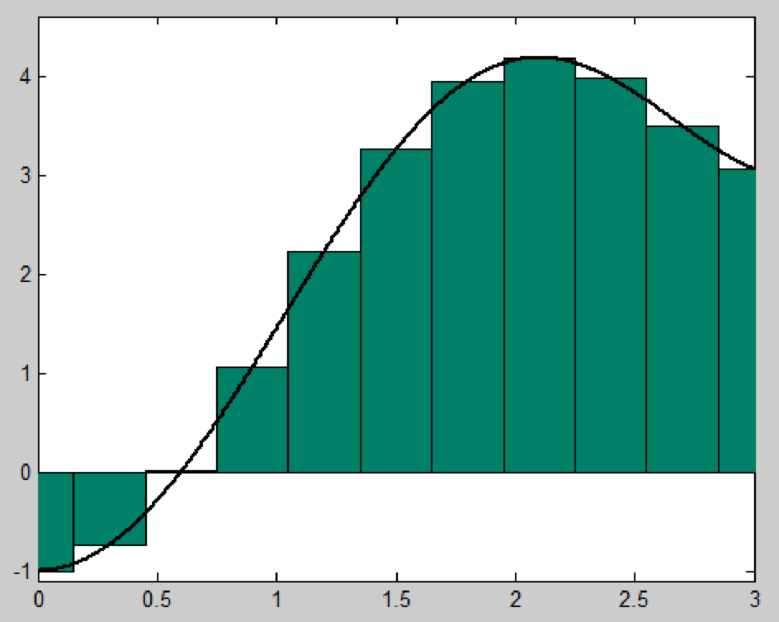
Richardson extrapolation and Romberg integration

Gaussian quadrature

Riemann integration

This is the simplest approach, and comes from Riemann's definition of integration, as the limit of a sum over *intervals of length* Δx*:*

$$\int_a^b f(x)\mathrm{d}x = \lim_{n\to\infty}\sum_{i=1}^{n} f(x_i)\Delta x$$



Riemann integration:

1. Divide the interval [a,b] into n subsegments of length

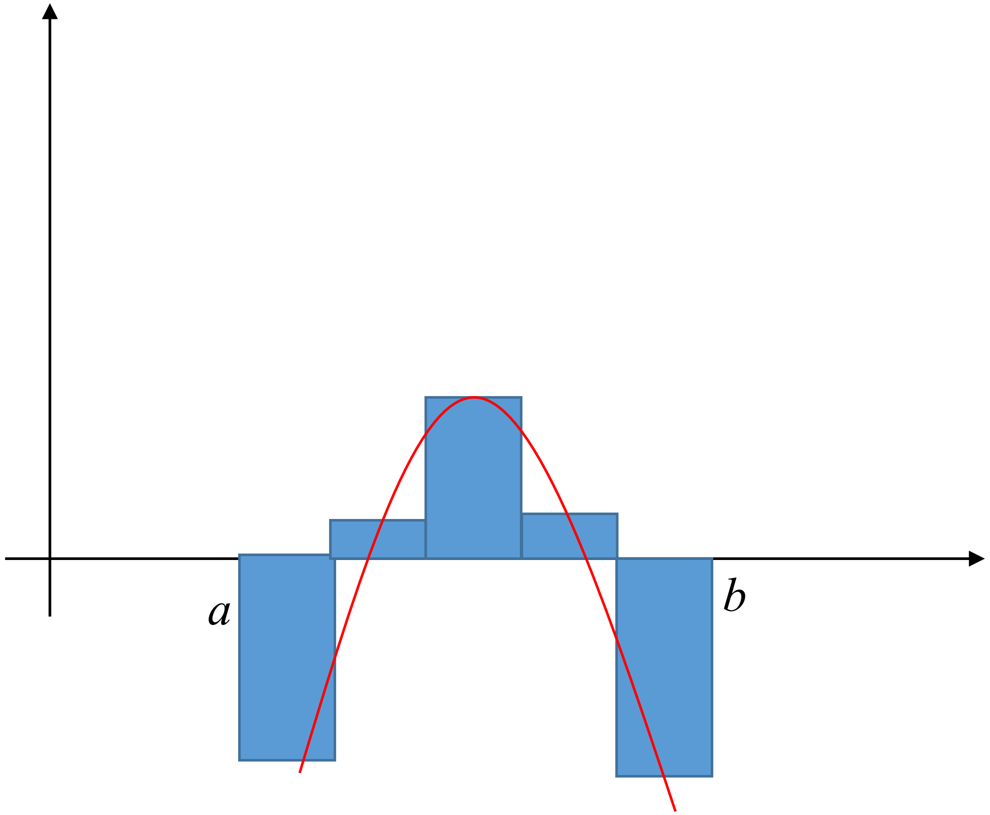
$$h = \frac{b-a}{n}$$

2. Perform the sum

$$\int_a^b f(x)\mathrm{d}x \approx \sum_{j=0}^{n-1} f(a+(j+1/2)h)h$$

This algorithm is

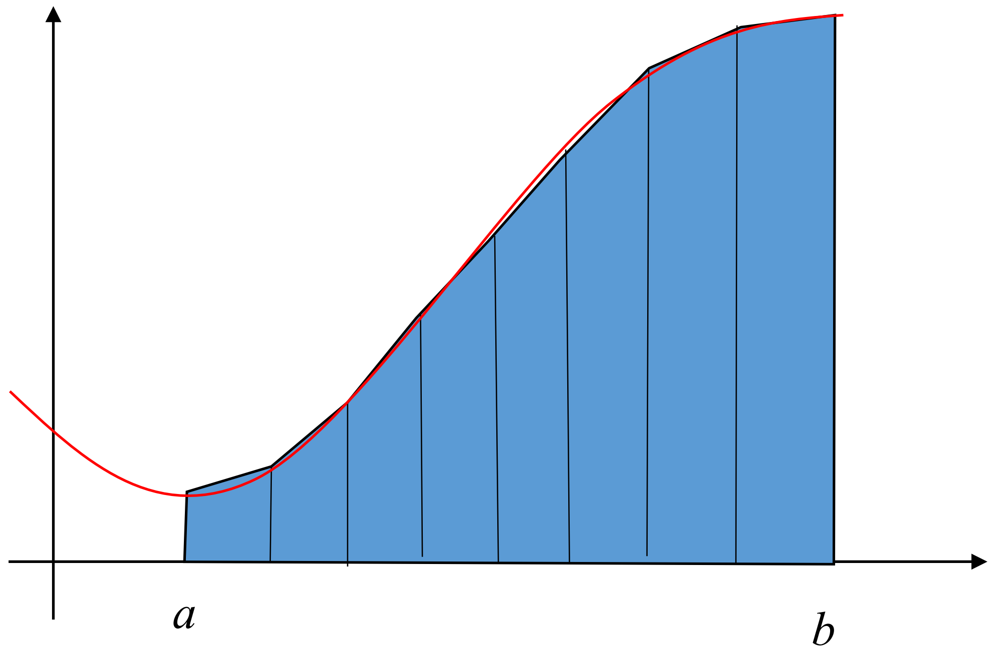
- Really quick to code
- Really bad (the error is of order $O(h^0)$!!).



The trapezoidal rule

This is the “rule of choice” for anything you need done quickly.

The idea: Break the interval up n into equal intervals (“panels”), then sum the areas of the trapezoids.



Area of each trapezoid:

The trapezoidal rule:

1. Break the interval into n panels of length

$$h = \frac{b-a}{n}$$

with nodes at $x_j = a + jh$, and function values $f_j = f(x_j)$

2. Form the sum

$$I = \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n\right)$$

The error in this method is *quadratic: that is,*

$$I = I_{\text{exact}} + O(h^2)$$

Simpson's rule: (we will derive this later)
This rule involves interpolating by a *parabola* rather than a line.

Simpson's rule:

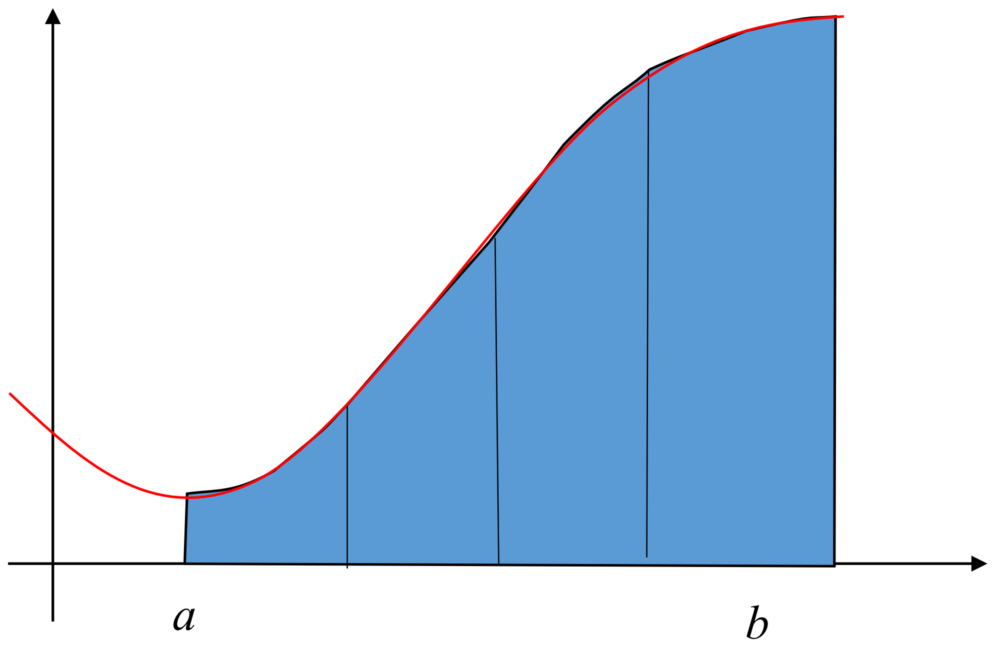
1. Break the interval into n panels of length

$$h = \frac{b-a}{n}$$

with nodes at $x_j = a + jh$, and function values $f_j = f(x_j)$

2. Form the sum

$$I = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + f_n\right)$$



The error in this method is *quartic: that is,*

$$I = I_{\text{exact}} + O(h^4)$$

The trapezoidal rule:

1. Break the interval into n panels of length

$$h = \frac{b-a}{n}$$

with nodes at $x_j = a + jh$, and function values $f_j = f(x_j)$

2. Form the sum

$$I = \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n\right)$$

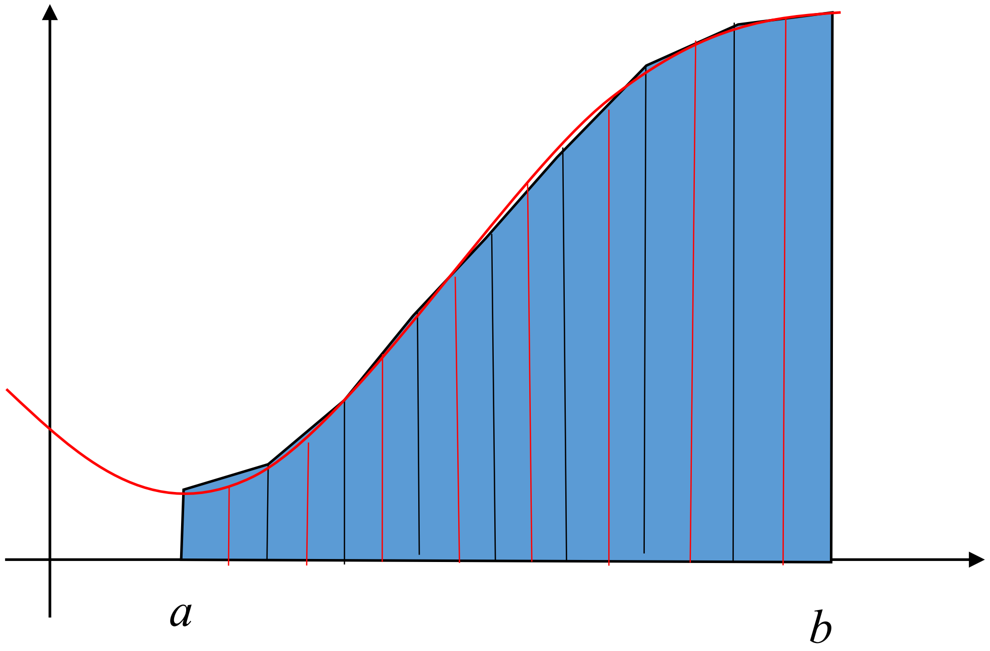
The error in this method is *quadratic: that is,*

$$I = I_{\text{exact}} + O(h^2)$$

What if we want to work out the integral *to within a given tolerance?*

The refined trapezoidal rule

This is a great “workhorse” numerical method. The idea is that you start with a quadrative interpolation, then keep inserting points until the required tolerance is reached.



$$I_n = \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n\right)$$

$$I_{2n} = \frac{h}{4}\left(f_0 + 2f_{\mathrm{i},1} + 2f_1 + 2f_{\mathrm{i},2} + 2f_2 + \cdots + 2f_{n-1} + 2f_{\mathrm{i,n}} + f_n\right)$$

Refining trapezoid algorithm

1. Compute the trapezoidal rule with n panels and interval size h_n

$$I_n = \frac{h_n}{2}\left(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n\right)$$

2. Compute the nodes of the intermediate points

$$x_{\mathrm{i},j} = \frac{1}{2}(x_j + x_{j+1}) \quad , j = \{1 \ldots n\}$$

3. Form the new integral, stop if converged

$$I_{2n} = \frac{1}{2} I_n + \frac{h_n}{2} \sum_{j=1}^{n} f(x_{\mathrm{i},j})$$

4. Merge the intermediate points $x_{\mathrm{i},j}$ with the set of nodes x_j,

5. Set $h_{2n} = h_n/2$ and repeat from Step 2.

Richardson extrapolation

The trapezoidal rule is an *approximation* to the exact value of the integral. That is,

$$I_{\mathrm{T}} = I_{\mathrm{exact}} + \mathrm{Error}(h)$$

We can show that the error is *quadratic in h*, that is

$$I_{\mathrm{T}} = I_{\mathrm{exact}} + c_1 h^2 + O(h^4)$$

We can derive *new rules of integration* by trying to cancel out this error.

To see how this works, let's see what happens when we halve the stepsize h:

We have found a new rule:

$$I_{\text{new}} = \frac{1}{3}\left[4I_{\text{T}}(h/2) - I_{\text{T}}(h)\right]$$

What does this look like?

Can we design higher order schemes? The answer is yes - This is called Romberg integration

$$I_1(h) = I_{\mathrm{T}}(h)$$

$$I_2(h) = \frac{1}{3}\left[I_1(\frac{h}{2}) - I_1(h)\right]$$

Now,

$$I_2(h) = I_{\text{exact}} + c_2 h^4$$

$$I_2(\frac{h}{2}) = I_{\text{exact}} + c_2 \left(\frac{h}{2}\right)^4$$

In general

$$I_j(h) = I_{\text{exact}} + c_j h^{2j}$$

$$I_j(\frac{h}{2}) = I_{\text{exact}} + c_j \left(\frac{h}{2}\right)^{2j}$$

$$\Rightarrow \quad I_{j+1}(h) = \frac{1}{2^{2j}-1}\left[2^{2j} I_j(\frac{h}{2}) - I_j(h)\right]$$

Higher-order quadrature schemes can be derived from the trapezoidal rule. Each iteration pushes the error out to a higher order in h.

Romberg integration

1. Compute the integral according to the trapezoidal rule with stepsize h, and 2 panels

$$R(n,0) = I_T(h)$$

2. While the integral is not converged:

- Set new panel size $$h_n = \frac{b-a}{2^n}$$
- Compute the integral according to the trapezoidal rule with stepsize h/2, 2n panels

$$R(n+1,0) = I_T(h_{n+1})$$

$$R(n+1,j) = \frac{1}{2^{2j}}\left[2^{2j}R(n+1,j-1) - R(n,j-1)\right] \quad j = 1...n+1$$

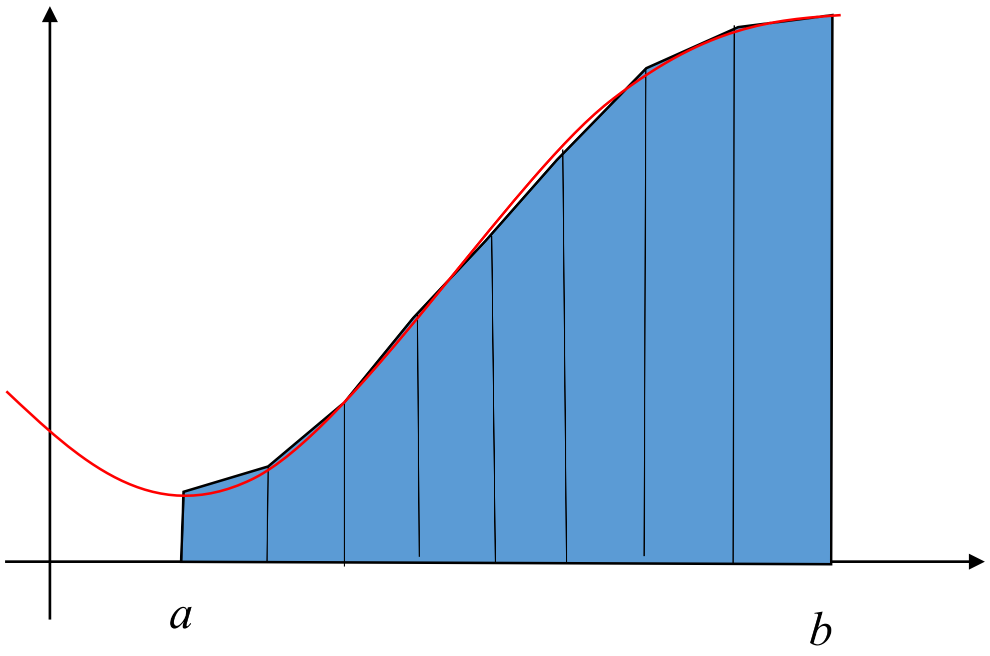
- Update n = n+1. The final term $I = R(n,n)$ is the value of the integral.

Gaussian Quadrature

All our quadrature schemes thus far have involved picking Equally-space points. In each case we have ended up with a formula like

$$I = \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n\right)$$

$$= \frac{h}{2}f_0 + 2\frac{h}{2}f_1 + 2\frac{h}{2}f_2 + \cdots + 2\frac{h}{2}f_{n-1} + \frac{h}{2}f_n$$



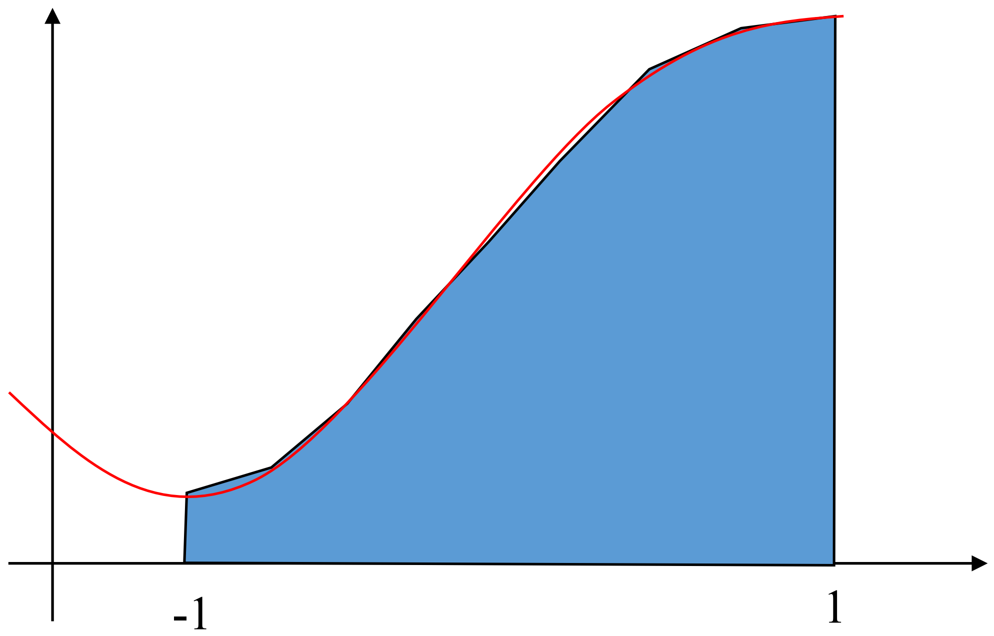
We can get faster, more accurate integrals if we are *free to pick our points as we like.* This idea leads to Gaussian quadrature.

Important point: Most Gaussian quadrature schemes are derived for the interval [-1,1].
We’ll do the change of variables later.

Imagine that we pick a set of points x_j. We can approximate our function by Lagrange interpolation:

$$f(x) \approx \sum_{j}^{n} \ell_j(x) f_j$$

Note that when f is a polynomial of order <n, this approximation is *exact.*



Integrating, we find

$$\ell_j(x) = \frac{\prod_{i \neq j}(x - x_i)}{\prod_{i \neq j}(x_j - x_i)}$$

How do we choose the points x_j? It turns out that a *really, really good choice* is that we choose them to be the zeros of orthogonal polynomials.

Orthogonal polynomials

Consider a set of polynomials $p_j(x)$ of degree 1…n. We say that This set is *orthogonal over an interval* [-1,1] if

$$\int p_i(x)p_j(x)w(x)\mathrm{d}x = 0 \quad \text{for } i \neq j$$

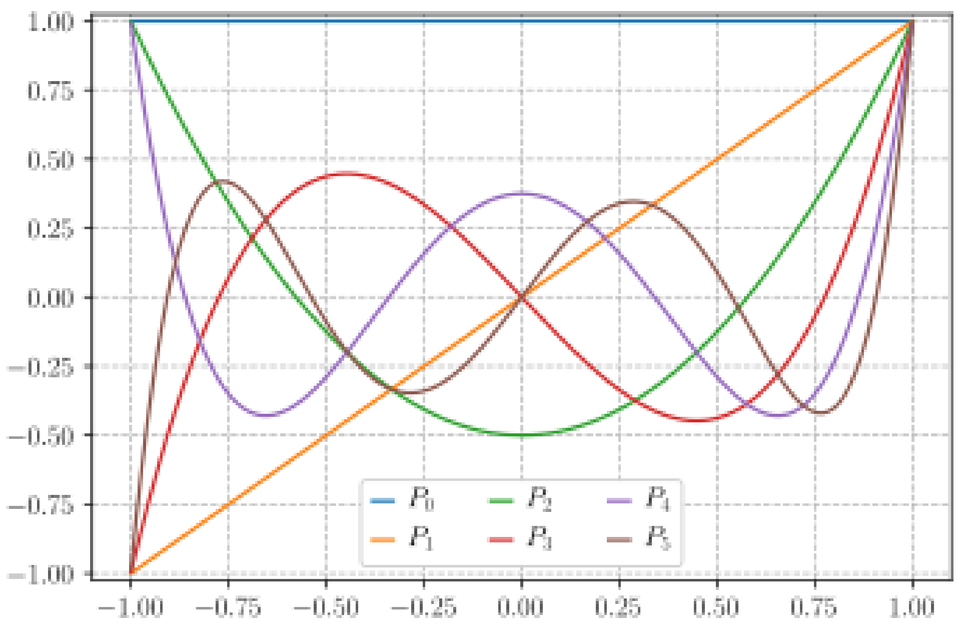
The type of polynomial depends on the weight function w(x):

Legendre polynomials

Chebyshev polynomials
(1st and second kind)

Jacobi polynomials

All these have been computed and their zeros tabulated



n	$P_n(x)$
0	1
1	x
2	$\frac{1}{2}(3x^2-1)$
3	$\frac{1}{2}(5x^3-3x)$
4	$\frac{1}{8}(35x^4-30x^2+3)$
5	$\frac{1}{8}(63x^5-70x^3+15x)$
6	$\frac{1}{16}(231x^6-315x^4+105x^2-5)$
7	$\frac{1}{16}(429x^7-693x^5+315x^3-35x)$
8	$\frac{1}{128}(6435x^8-12012x^6+6930x^4-1260x^2+35)$
9	$\frac{1}{128}(12155x^9-25740x^7+18018x^5-4620x^3+315x)$
10	$\frac{1}{256}(46189x^{10}-109395x^8+90090x^6-30030x^4+3465x^2-63)$

Once we have the polynomials, we can look up the zeros and the weights, and evaluate

$$\int_{-1}^{1} f(x)w(x)\mathrm{d}x \approx \sum_{j=1}^{n} w_j f(x_j)$$

Number of points, n	Points, x_i		Weights, w_i	
1	0		2	
2	$\pm\frac{1}{\sqrt{3}}$	±0.57735...	1	
3	0		$\frac{8}{9}$	0.888889...
	$\pm\sqrt{\frac{3}{5}}$	±0.774597...	$\frac{5}{9}$	0.555556...
4	$\pm\sqrt{\frac{3}{7}-\frac{2}{7}\sqrt{\frac{6}{5}}}$	±0.339981...	$\frac{18+\sqrt{30}}{36}$	0.652145...
	$\pm\sqrt{\frac{3}{7}+\frac{2}{7}\sqrt{\frac{6}{5}}}$	±0.861136...	$\frac{18-\sqrt{30}}{36}$	0.347855...
5	0		$\frac{128}{225}$	0.568889...
	$\pm\frac{1}{3}\sqrt{5-2\sqrt{\frac{10}{7}}}$	±0.538469...	$\frac{322+13\sqrt{70}}{900}$	0.478629...
	$\pm\frac{1}{3}\sqrt{5+2\sqrt{\frac{10}{7}}}$	±0.90618...	$\frac{322-13\sqrt{70}}{900}$	0.236927...

We usually have to *change the interval* of integration. This involves the change of coordinates

$$\int_{a}^{b} f(x)\mathrm{d}x = \int_{-1}^{1} f\left(\frac{b-a}{2}u + \frac{a+b}{2}\right)\frac{dx}{du}du$$

$$\int_{a}^{b} f(x)w(x)\mathrm{d}x \approx \frac{b-a}{2}\sum_{j=1}^{n} w_j f\left(\frac{b-a}{2}u_j + \frac{a+b}{2}\right)$$

Gaussian quadrature

To integrate functions of the type

$$\int_a^b f(x)w(x)\mathrm{d}x$$

1. Choose an appropriate set of polynomials for the weighting,
and the number of points n at which you are using to integrate the function

2. Evaluate the sum

$$\int_a^b f(x)w(x)\mathrm{d}x \approx \frac{b-a}{2}\sum_{j=1}^{n} w_j f\left(\frac{b-a}{2}x_j + \frac{a+b}{2}\right)$$

where the w_j and x_j are the tabulated weights and zeros for the expansion.

Gaussian quadrature is

1. Simple to implement

2. Extremely fast

3. More accurate (by far) than almost any other method

Why Gaussian quadrature works so well