Numerical Methods

DS288 and UMC201

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August-December 2025

Composite Trapezoidal rule

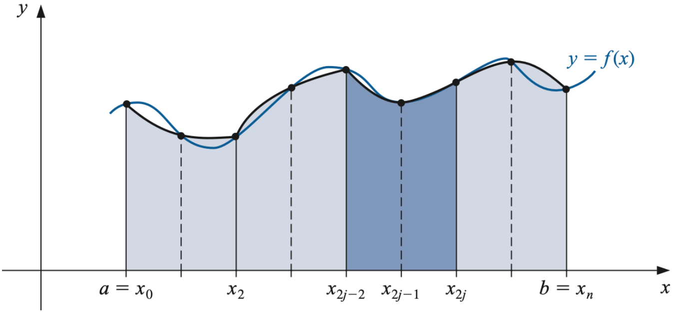
- Let $f \in C^2[a,b]$, $h = (b-a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \cdots, n$.
- There exists $\mu \in (a,b)$ for which the Composite Trapezoidal rule for n sub-intervals can be written with its error term as

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu)$$

Composite Simpson's rule

- Let $f \in C^4[a, b]$, n be even, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \cdots, n$.
- There exists $\zeta \in (a, b)$ for which the Composite Simpson's rule for n sub-intervals can be written with its error term as

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} + f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180}h^4 f^{(4)}(\zeta)$$



Example

Example

Determine values of h that will ensure approximation error of less than 0.00002 while approximating $\int_0^{\pi} \sin(x)dx$ on $[0, \pi]$ using (a). Composite Trapezoidal rule and (b): Composite Simpson's rule.

(a): Composite Trapezoidal rule

- Error: $\left|\dfrac{\pi h^2}{12} f''(\mu)\right| = \dfrac{\pi h^2}{12} |\sin(\mu)| \leq \dfrac{\pi h^2}{12} < 0.00002$
- since $h = \pi/n$. Thus $n = \pi/h$, we need $\frac{\pi^3}{12n^2} < 0.00002$
- $n \geq \left(\frac{\pi^3}{12(0.00002)}\right)^{1/2} = 359.44 \approx 360$

(b): Composite Simpson's rule

- Error: $|\dfrac{\pi h^4}{180} f^{(4)}(\mu)| = \frac{\pi h^4}{180} |\sin(\mu)| \leq \frac{\pi h^4}{180} < 0.00002$
- $h \leq 0.18398$, $n \geq 18$

Best Choice for h

- Approximation error is of the form ch^p which $\to 0$ as $h \to 0$.
- The approximation $f^{(r)}(x)$ contains h^r in the denominator.
- As h is successively decreased to smaller values, the truncation error decreases, but the round-off error in the method may increase as we are dividing by a small number.
- It may happen that after a certain critical value of h, the round-off error may become more dominant than the truncation error and the numerical results obtained may start worsening as h is further reduced.
- when $f(x)$ is given in tabular form, these values may not themselves be exact. These values contain round-off error, i.e.,

$$f(x_i) = f_i + \epsilon_i, \text{ where } f(x_i): \text{ exact value, } f_i: \text{ tabulated value}$$

Choice for h

- To see effect of the round-off error, we consider

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{h} - \frac{h}{2} f''(\zeta), \quad x_0 < \zeta < x_1$$

- If the round off error in $f(x_0)$ and $f(x_1)$ and ϵ_0 and ϵ_1 respectively. Then we have

$$\begin{aligned} f'(x_0) &= \frac{f_1 - f_0}{h} + \frac{\epsilon_1 - \epsilon_0}{h} - \frac{h}{2} f''(\zeta) \\ f'(x_0) &= \frac{f_1 - f_0}{h} + \text{RE(round-off error)} + \text{TE(truncation error)} \end{aligned}$$

- If we take $\epsilon = \max(|\epsilon_1|, |\epsilon_2|)$ and $M_2 = \max\limits_{x_0 \le x \le x_1} |f''(x)|$

- Then we get $|RE| \le \dfrac{2\epsilon}{h}$, $|TE| \le \dfrac{h}{2} M_2$

- Optimal value of h depends on one of the following criteria

(i) $|RE| = |TE|$ or (ii) $|RE| + |TE| = \text{minimum}$

Choice for h

- Optimal value of h depends on one of the following criteria

  (i) $|RE| = |TE|$
  (ii) $|RE| + |TE| = \text{minimum}$

- Following first condition, (i), we have $\dfrac{2\epsilon}{h} = \dfrac{h}{2}M_2$
- This gives $h_{adaptive} = 2\sqrt{\epsilon/M_2}$
- Following first condition, (ii), we have

$$\frac{2\epsilon}{h} + \frac{h}{2}M_2 = \text{minimum}, \quad \Rightarrow -\frac{2\epsilon}{h^2} + \frac{1}{2}M_2 = 0 \tag{1}$$

- Thus $h_{adaptive} = 2\sqrt{\epsilon/M_2}$

Example

Example

For the following method, determine the optimal value of h

$$f'(x) = \frac{-3f(x_0) + 4f(x_1) - f(x_2)}{2h} + \frac{h^2}{3} f'''(\zeta), \;\; x_0 < x < x_2$$

Consider $f(x) = ln(x)$ with tabular value.

x	2.0	2.01	2.02	2.06	2.12
$f(x)$	0.69315	0.69813	0.70310	0.72271	0.75142

with given maximum round-off error in function evaluation is 5×10^{-6}

Section-4.2
Richardson's Extrapolation

Richardson's Extrapolation

- Taylor Series of f about the point x and evaluated at $x+h$ and $x-h$ leads to the central difference formula:
- Solving for f_j' gives: $f_j' = \dfrac{f_{j+1} - f_{i-1}}{2h} + O(h^2)$
- This formula describes precisely how the error behaves.
- This information can be exploited to improve the quality of the numerical solution without ever knowing $f^{(3)}, f^{(5)}, \cdots$
- Let us rewrite this in the following form:

$$f_j' = N_1(h) - \frac{h^2}{6} f_j''' - \frac{h^4}{120} f_j^{(5)} - \cdots$$

where $N_1(h) = \frac{f(x+h) - f(x-h)}{2h}$

- The key of the process is to now replace h by $h/2$ in this formula

Richardson's Extrapolation

- Richardson's extrapolation is used to generate high-accuracy results while using low-order formulas.
  - When an approximation technique has an error term with a predictable form
  - Which depends on a parameter (say, step size h)

Let we have an approximation formula $N_1(h)$ that approximates an unknown constant M

- The truncation error

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

  where $K_1, K_2, K_3, \ldots$ are unknown constants
- The truncation error is $\mathcal{O}(h)$, i.e., $M - N_1(h) \approx K_1 h$.

Richardson's Extrapolation

- Let $N_2(h)$ is an $\mathcal{O}(h^2)$ approximation formula (obtained by taking a combination of $N_1(h)$ approximations) for M with

$$M - N_2(h) = \hat{K}_2 h^2 + \hat{K}_3 h^3 + \cdots ,$$

  such that $M - N_2(h) \approx \hat{K}_2 h^2$.
- $N_2(h)$ is a better approximation than $N_1(h)$, provided K_1 and $\hat{K}_2$ are comparable in the magnitude.
- Similarly, by taking a combination of $N_2(h)$, we can obtain a third order approximation formula $N_3(h)$, such that, $M - N_3(h) \approx \hat{\hat{K}}_3 h^3$.

Richardson's Extrapolation

How to generate the extrapolation formulas?

- Let $M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$
- The above expression is also true for $h/2$, i.e.,
$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h}{2} + K_2\frac{h^2}{4} + K_3\frac{h^3}{8} + \cdots$$
- Subtracting the first equation with twice of the second equation, we get
$$M = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots$$
- Hence, we have an $\mathcal{O}(h^2)$ approximation formula for M, i.e., $M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots$, where
$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right].$$

Example

Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1$, and $h = 0.05$. Further, use extrapolation on these values

- first-order approximation formula $N_1(h)$ based on forward-difference
- Use $\dfrac{d}{dx}(\ln x) = \dfrac{1}{x}$, we get $f'(1.8) = 1/1.8 = 0.\overline{5}$.
- for $h = 0.1$, $f'(1.8) \approx \dfrac{f(1.9) - f(1.8)}{0.1} = 0.5406722 = N_1(0.1)$ with error 1.5×10^{-2}
- for $h = 0.05$, $f'(1.8) \approx \dfrac{f(1.85) - f(1.8)}{0.05} = 0.5479795 = N_1(0.05)$ with error 7.7×10^{-3}
- Extrapolating these two results to obtain the new approximation

$$N_2(0.1) = N_1(0.05) + (N_1(0.05) - N_1(0.1)) = 0.555287$$

with error 2.7×10^{-4}.

Richardson's Extrapolation

- Extrapolation can be applied whenever the truncation error for a formula has the form $\sum_{j=1}^{m-1} K_j h^{\alpha_j} + \mathcal{O}(h^{\alpha_m})$ for constants K_j and $\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m$.
- Some extrapolation formulas have truncation errors with only even powers of h, $M = N_1(h) + K_1 h^2 + K_2 h^4 + \cdots$.
- Subtracting the above equation from four times the equation $M = N_1\left(\frac{h}{2}\right) + K_1 \frac{h^2}{4} + K_2 \frac{h^4}{16} + \cdots$, we get

$$M = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + \frac{K_2}{3}\left(\frac{h^2}{4} - h^4\right) + \frac{K_3}{3}\left(\frac{h^6}{16} - h^6\right) + \cdots$$

- gives us the fourth-order approximation formula

$$N_2(h) = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] = N_1\left(\frac{h}{2}\right) + \frac{1}{3}\left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]$$

Section-4.5
Romberg Integration

Romberg Integration

- For $f \in C^{\infty}[a, b]$, the composite Trapezoidal rulde can be written with an error term in the form

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] + K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots$$

Where constant K_i are depends only on $f^{(2i-1)}(a)$ and $f^{(2i-1)}(b)$

- Here the truncation error has the form

$$\sum_{j=1}^{m-1} K_j h^{2j} + \mathcal{O}(h^{2m}).$$

- Therefore, Richardson extrapolation can be performed.

Romberg Integration

- Use the results of the Composite Trapezoidal rule with $n = 1, 2, 4, 8, 16, \ldots$ to approximate the integral $\int_a^b f(x)dx$, denoted by $R_{1,1}, R_{2,1}, R_{3,1}, \ldots,$ respectively.
- Then obtain $\mathcal{O}(h^4)$ approximations $R_{2,2}, R_{3,2}, R_{4,2}, \ldots,$ where

$$R_{k,2} = R_{k,1} + \frac{1}{3}(R_{k,1} - R_{k-1,1}), \quad \text{for } k = 2, 3, \ldots$$

- Then the $\mathcal{O}(h^6)$ approximations $R_{3,3}, R_{4,3}, R_{5,3}, \ldots$

$$R_{k,3} = R_{k,2} + \frac{1}{15}(R_{k,2} - R_{k-1,2}), \quad \text{for } k = 3, 4, \ldots$$

- In general, to obtain the $\mathcal{O}(h^{2j})$ approximations $R_{k,j-1}$

$$R_{k,j} = R_{k,j-1} + \frac{1}{4^{j-1} - 1}(R_{k,j-1} - R_{k-1,j-1}), \quad \text{for } k = j, j+1, \ldots$$

Example

- To find approximations to $\int_0^{\pi} \sin x dx$, with $n = 1, 2, 4, 8, 16$

$$R_{1,1} = \frac{\pi}{2}[\sin 0 + \sin \pi] = 0$$

$$R_{2,1} = \frac{\pi}{4}\left[\sin 0 + 2\sin\frac{\pi}{2} + \sin \pi\right] = 1.57079633$$

$$R_{3,1} = \frac{\pi}{8}\left[\sin 0 + 2\left(\sin\frac{\pi}{4} + \sin\frac{\pi}{2} + sin\frac{3\pi}{4}\right) + \sin \pi\right] = 1.8961189$$

$$R_{4,1} = 1.97423160$$

$$R_{5,1} = 1.99357034.$$

- Then using Romberg integration, we obtain the $\mathcal{O}(h^4)$ approximations

$$R_{2,2} = R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1}) = 2.09439511, \quad R_{3,2} = 2.00455976$$

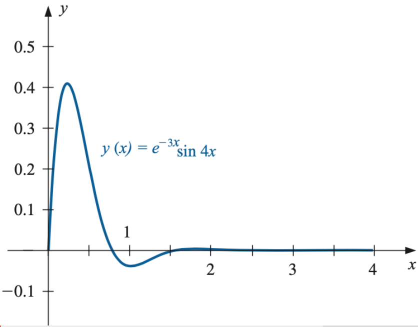
$$R_{4,2} = 2.00026917, \quad R_{5,2} = 2.00001659.$$

Section-4.6
Adaptive Quadrature Methods

Adaptive Quadrature Methods

- Composite formulas suffer occasionally, since they require the use of equally-spaced nodes
- Inappropriate for functions having different regions of large and small functional variations

Example: The solution of the differential equation $y'' + 6y' + 25 = 0$, with $y(0) = 0$ and $y'(0) = 4$ is $y(x) = e^{-3x} \sin 4x$.



Adaptive Quadrature Methods

- To approximate $\int_a^b f(x)dx$, within a tolerance $\varepsilon > 0$
- Use Simpson's rule with step size $h = (b-a)/2$

$$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\xi), \quad \text{for some } \xi \in (a,b) \qquad (2)$$

where the Simpson's rule approximation is

$$S(a,b) = \frac{h}{3}[f(a) + 4f(a+h) + f(b)]$$

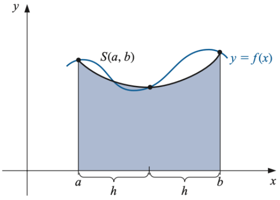
Adaptive Quadrature Methods

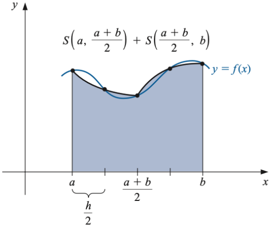
- Next, to determine an accuracy approximation that does not require $f^{(4)}(\xi)$, using Composite Simpson's rule with $N = 4$ and step size $(b-a)/4 = h/2$, giving

$$\int_a^b f(x)dx \approx \frac{h}{6}\left[f(a) + 4f\left(a+\frac{h}{2}\right) + 2f(a+h) + 4f\left(a+\frac{3h}{2}\right) + f(b)\right] \tag{3}$$

$$\approx S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)$$

with error $-\frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\xi})$, for some $\tilde{\xi} \in (a, b)$.





Adaptive Quadrature Methods

- From (2) and (3) with $\zeta \approx \tilde{\zeta}$ we get

$$S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi) \approx S(a,b) - \frac{h^5}{90} f^{(4)}(\xi)$$

This implies

$$\frac{h^5}{90} f^{(4)}(\xi) \approx \frac{16}{15}\left[S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right]$$

Adaptive Quadrature Methods

- The above estimate (3) produces the error estimation

$$\left|\int_a^b f(x)dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \approx \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi)$$
$$\approx \frac{1}{15}\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right|$$

- Implies that

$$\left|S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - S(a,b)\right| < 15\varepsilon$$

Therefore, $S(a,(a+b)/2) + S((a+b)/2, b)$ approximates $\int_a^b f(x)dx$ with a sufficient accuracy, such that,

$$\left|\int_a^b f(x)dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < \varepsilon.$$

Example

- For the integral $\int_0^{\pi/2} sinx dx = 1$.
- We have
$$S\left(0, \frac{\pi}{2}\right) = \frac{\pi/4}{3}\left[sin0 + 4sin\frac{\pi}{4} + sin\frac{\pi}{2}\right] = 1.002279878$$
- and
$$S\left(0, \frac{\pi}{4}\right) - S\left(\frac{\pi}{4}, \frac{\pi}{2}\right) = 1.000134585$$
- Therefore,
$$\left|S\left(0, \frac{\pi}{4}\right) + S\left(\frac{\pi}{4}, \frac{\pi}{2}\right) - S\left(0, \frac{\pi}{2}\right)\right| = 0.002145293$$
- Hence, the estimate of the error obtained using $S(a, (a+b)/2) + S((a+b)/2, b)$ to approximate $\int_a^b f(x)dx$ is
$$\frac{1}{15}\left|S\left(0, \frac{\pi}{4}\right) - S\left(\frac{\pi}{4}, \frac{\pi}{2}\right) - S\left(0, \frac{\pi}{2}\right)\right| = 0.000143020.$$

Numerical Integration

Method of Undetermined Coefficients

- Consider the integral $\int_a^b f(x)\,dx = A_0 f(a) + A_1 f(b) + \alpha f''(\beta)$ where A_0, A_1, α are unknowns and are to be found.
- Taking $f(x) = 1 \Rightarrow b - a = A_0 + A_1$
  $f(x) = x \Rightarrow \dfrac{b^2 - a^2}{2} = A_0 a + A_1 b$
- On solving these two equations, we get
  $A_0 = A_1 = \dfrac{b-a}{2}$

Numerical Integration

Method of Undetermined Coefficients (Trapezoidal rule)

- Thus the integration rule becomes
$$\int_a^b f(x)\,dx = \frac{b-a}{2}[f(a)+f(b)] + \alpha f''(\beta)$$
- Take $f(x) = x^2 \Rightarrow \dfrac{b^3 - a^3}{3} = \left(\dfrac{b-a}{2}\right)(a^2 + b^2) + 2\alpha$

  This gives $\alpha = -\dfrac{(b-a)^3}{12}$
- Therefore, we get
$$\int_a^b f(x)\,dx = \frac{b-a}{2}[f(a)+f(b)] - \frac{(b-a)^3}{12} f''(\beta)$$
which is the basic Trapezoidal rule with error term.

Numerical Integration

Method of Undetermined Coefficients (Simpson's 3/8 rule)

- **Example:** Simpson's 3/8 rule by method of undetermined coefficients.
- Consider the integral

  $$\int_{x_0}^{x_3} f(x)\,dx = A_0 f_0 + A_1 f_1 + A_2 f_2 + A_3 f_3 + \alpha f^{(4)}(\beta) \text{ for some } \beta \in (x_0, x_3)$$

- With out loss of generality taking $x_0 = 0$, $x_1 = h$, $x_2 = 2h$, $x_3 = 3h$ and $f(x) = 1$, x, x^2, x^3, x^4 in the above integral to get

  $$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}[f_0 + 3f_1 + 3f_2 + f_3] - \frac{3h^5}{80} f^{(4)}(\beta)$$

Numerical Integration: Gaussian Quadrature

- All the Newton-Cots formulas use values of the function at equally spaced points.
- Gaussian quadrature chooses the points for evolution in an optimal way rather than equally spaced.
- Select functional values at non-uniformly distributed points to achieve higher accuracy.
- The nodes $x_1, x_2, \cdots, x_n$ in the interval $[a, b]$ and coefficients $c_1, c_2, \cdots c_n$ are chosen to minimize the expected error obtained in the approximation.

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i)$$

Numerical Integration: Gaussian Quadrature

- That is, we look for numerical integration formulas which are to be exact for polynomials as large a degree as possible.
- The coefficients $c_1, c_2, \cdots c_n$ are arbitrary and the nodes $x_1, x_2, \cdots x_n$ are restricted only in the fact that they must lie in $[a, b]$, the interval of the integration. This gives $2n$ parameters to choose.
- If coefficients of a polynomial are considered as parameters, the class of polynomials of degree at most $(2n - 1)$ also contains $2n$ parameter.
- Therefore this is the largest class of polynomials for which it is reasonable to expect the exact formula to be exact.
- For example, first we will show how to select the coefficients and nodes when n=2 and the interval of integration is [-1, 1].
- Later, we discuss the more general situation for an arbitrary choice of nodes and coefficients and how the method is modified when the integration over an arbitrary interval.

Numerical Integration

Gaussian Quadrature on $[-1, 1]$

- Suppose we want to find c_1, c_2, x_1 and x_2 (i.e. $n = 2$) so that the integration formula

$$n = 2: \quad \int_{-1}^{1} f(x)\,dx \cong c_1 f(x_1) + c_2 f(x_2)$$

gives exact result whenever $f(x)$ is a polynomial of degree $2.2 - 1 = 3$ or less.

Numerical Integration: Gaussian Quadrature

- Hence choose c_1, c_2, x_1, x_2 such that the method yields *exact integral* for $f(x) = x^0, x^1, x^2, x^3$. That is

$$\begin{cases} f = 1 \Rightarrow \int_{-1}^{1} 1\,dx = 2 = c_1 + c_2 \\ f = x \Rightarrow \int_{-1}^{1} x\,dx = 0 = c_1x_1 + c_2x_2 \\ f = x^2 \Rightarrow \int_{-1}^{1} x^2\,dx = \frac{2}{3} = c_1x_1^2 + c_2x_2^2 \\ f = x^3 \Rightarrow \int_{-1}^{1} x^3\,dx = 0 = c_1x_1^3 + c_2x_2^3 \end{cases} \Rightarrow \begin{cases} c_1 = 1 \\ c_2 = 1 \\ x_1 = -\frac{1}{\sqrt{3}} \\ x_2 = \frac{1}{\sqrt{3}} \end{cases}$$

- Therefore, we get the formula

$$\boxed{\int_{-1}^{1} f(x)\,dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)}$$

Gaussian Quadrature(The General Case)

- We want to find the weights c_i and nodes x_i $(i = 1, 2, ..., n)$, so as to have

$$\int_{-1}^{1} f(x)\,dx \cong \sum_{i=1}^{n} c_i f(x_i)$$

  be exact for polynomials $f(x)$ of degree as large as possible.
- $2n$ unknowns so need $2n$ equations to find these unknowns.
- We require the quadrature formula to be exact for the cases $f(x) = x^i$ for $i = 0, 1, 2, ..., 2n - 1$.
- Then we obtain the system of non linear equations

$$c_1 x_1^i + c_2 x_2^i + c_3 x_3^i + ... + c_n x_n^i = \int_{-1}^{1} x^i\,dx \quad \text{for } i = 0, 1, 2, ..., 2n - 1.$$

Gaussian Quadrature

- The right side values are

$$\int_{-1}^{1} x^i \, dx = \begin{cases} \dfrac{2}{i+1} & \text{for } i = 0, 2, 4, ..., 2n-2 \\ 0 & \text{for } i = 1, 3, 5, ..., 2n-1. \end{cases}$$

- The system of $2n$-equations is to be solved uniquely.
- The resulting numerical integration rule is called **Gaussian Quadrature**.


ANY
QUESTIONS?