Set 17: Newton-Cotes Quadrature

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Numerical Quadrature

Let $f(x) \in \mathcal{C}[a,b]$. Numerical quadrature approximates the definite integral

$$I_n(f) \approx \int_a^b f(x)dx$$

$$I_n(f) = I(f_n) = \int_a^b f_n(x)dx$$

- $f_n(x)$ must be easy to integrate.
- $f_n(x) \approx f(x)$ and depends on $n \geq 0$.
- $f_n(x)$ could be a polynomial of degree n
- Lagrange, Hermite, Hermite-Birkhoff interpolation
- The text uses $I_n(f)$ where n is the degree and Isaason and Keller uses $I_{n+1}(f)$ for the same method, i.e., subscript is number of points.

Midpoint Rule

- Choose form of approximation: Lagrange interpolating polynomial
- Choose degree of interpolating polynomial: $n = 0$
- Choose interpolation point: $x_0 = (a + b)/2$
- $p_0(x) = f(x_0) = f_0$
- integrate to define method

$$I_0(f) = I(f_0) = \int_a^b f_0 dx = (b - a) f_0$$

Trapezoidal Rule

- Choose form of approximation: Lagrange interpolating polynomial
- Choose degree of interpolating polynomial: $n = 1$
- Choose interpolation points: $x_0 = a$, $x_1 = b$
- $p_1(x) = f(x_0) + (x - a)f[x_0, x_1]$
- integrate to define method

$$I_1(f) = I(f_1) = \int_a^b (f(x_0) + (x - a)f[x_0, x_1])\, dx$$

$$x = a + s(b - a), \quad dx = (b - a)ds$$

$$I_1(f) = (b - a) \int_0^1 (f_0 + s(f_1 - f_0))\, ds$$

$$= (b - a)\big[f_0 s + (f_1 - f_0)\frac{s^2}{2}\big]_0^1 = \frac{(b - a)}{2}(f_0 + f_1)$$

Simpson's Rule

Quadratic interpolant with uniform spacing $h = (b-a)/2$.

$$x_0 = a, \quad x_1 = a+h, \quad x_2 = a+2h = b$$

$$x = a + sh, \quad dx = h\,ds$$

$$I_2(f) = \int_a^b \left(f_0 + (x-x_0)f[x_0,x_1] + (x-x_0)(x-x_1)f[x_0,x_1,x_2]\right) dx$$

$$= h\int_0^2 \left(f_0 + shf[x_0,x_1] + (s)(s-1)h^2 f[x_0,x_1,x_2]\right) ds$$

Simpson's Rule

$$\pi_{k+1}(s) = \prod_{i=0}^{k}(s-i)$$

$$\begin{aligned}
I_2(f) &= h\int_0^2 \left(f_0 + \Delta f_0 \frac{\pi_1(s)}{1!} + \Delta^2 f_0 \frac{\pi_2(s)}{2!} \right) ds \\
&= h f_0 \left[s\right]_0^2 + h\Delta f_0 \left[\frac{s^2}{2}\right]_0^2 + h\frac{\Delta^2 f_0}{2}\left[\frac{s^3}{3} - \frac{s^2}{2}\right]_0^2 \\
&= h\left(2f_0 + 2\Delta f_0 + \frac{1}{3}\Delta^2 f_0\right) \\
&= h\left[\frac{1}{3}f_0 + \frac{4}{3}f_1 + \frac{1}{3}f_2\right]
\end{aligned}$$

Note. Note change in notation form earlier slides on divided differences for equidistant points, i.e., the subscript of $\pi(s)$.

Example

Compare three methods for $f(x) = e^x$.

$$I = \int_0^1 e^x dx = e - 1 = 1.718281828\ldots$$

$$h_0 = 0.5, \quad h_1 = 1.0, \quad h_2 = 0.5$$

$$I_0 = e^{0.5} = 1.648721271\ldots, \quad I_1 = \frac{e+1}{2} = 1.859140914\ldots$$

$$I_2 = \frac{1}{6}\left[1 + 4e^{0.5} + e\right] = 1.718861152\ldots$$

$$|I - I_0| = 0.069\ldots, \;\; |I - I_1| = 0.1408\ldots, \;\; |I - I_2| = 0.00058\ldots$$

Error comparison seems counterintuitive! $|I - I_0| < |I - I_1|$

Interpolatory Quadrature

Definition 17.1. Let $x_0, \ldots, x_n$ be $n+1$ distinct points. Given $f(x) \in \mathcal{C}[a,b]$, let $p_n(x)$ be the interpolating polynomial of degree n. The Lagrange interpolatory quadrature formula is given by

$$\begin{aligned} I_n(f) = I(p_n) &= \int_a^b p_n(x)dx \\ &= \int_a^b \{\sum_0^n \ell_{n,i}(x) f(x_i)\} dx \\ &= \sum_0^n \{\int_a^b \ell_{n,i}(x)\} f(x_i) dx \\ &= \sum_0^n \alpha_{n,i} f(x_i) dx \end{aligned}$$

Note. The subscript n on ℓ and α is dropped unless needed for clarity.

Numerical Quadrature

Definition 17.2. The degree of exactness or the degree of precision of a quadrature formula, $I_n(f)$, is the maximum integer m such that

$$I(x^k) - I_n(x^k) = 0 \quad 0 \le k \le m$$

$$I(x^{m+1}) - I_n(x^{m+1}) \neq 0$$

Definition 17.3. The order of infinitesimal of the quadrature formula $I_n(f)$ is the largest integer m such that $|I(f) - I_n(f)| = O(h^m)$.

Interpolatory Quadrature

We are not restricted to Lagrange interpolants. Hermite and any of the others can be used, but we have the following:

Theorem 17.1. *A quadrature formula using $n + 1$ distinct points is an interpolatory quadrature formula if and only if it has degree of exactness greater than or equal to n.*

Interpolatory Quadrature Error

Simple error bounds are easily deduced.

Lemma. *Let* $f(x) \in \mathcal{C}[a,b]$ *and* $E_n(f) = I(f) - I_n(f)$. *We have*

$$|E_n(f)| = |I(f) - I_n(f)|$$

$$= |\int_a^b f(x) - p_n(x) dx| \leq (b-a)\|f - p_n\|_\infty$$

and therefore

$$\|f - p_n\|_\infty \leq \epsilon \rightarrow |E_n(f)| \leq \epsilon(b-a)$$

Interpolatory Quadrature Error

Simple error bounds are easily deduced.

Lemma. *Let* $f(x) \in \mathcal{C}[a,b]$ *and* $E_n(f) = I(f) - I_n(f)$. *We have*

$$|E_n(f)| = |I(f) - I_n(f)|$$

$$= |\int_a^b \omega_n(x) f[x_0, x_1, \ldots, x_n, x] dx|$$

$$\leq \max_{a \leq x \leq b} |f[x_0, x_1, \ldots, x_n, x]| |\int_a^b \omega_n(x) dx|$$

Newton-Cotes Closed Formulas

- $n+1$ points in $[a,b]$ with $x_0 = a$ and $x_n = b$
- equally spaced points, $x_i = x_0 + ih_n, \;\; 0 \le i \le n$, i.e., $h_n = (b-a)/n$.
- coefficients depend only on n and h_n, i.e., precomputable
- degree of exactness is n when n is odd
- degree of exactness is $n+1$ when n is even, $\therefore$ odd number of points used typically
- for $n > 6$, coefficients get large and negative values appear (stability concerns)
- note form of error bound

Newton-Cotes Closed Formulas

$$I_1 : \frac{h_1}{2}\left[f_0 + f_1\right], \quad E_1 = -\frac{h_1^3}{12} f^{(2)}(\eta), \text{ trapezoidal rule}$$

$$I_2 : \frac{h_2}{3}\left[f_0 + 4f_1 + f_2\right], \quad E_2 = -\frac{h_2^5}{90} f^{(4)}(\eta), \text{ Simpson's first rule}$$

$$I_3 : \frac{3h_3}{8}\left[f_0 + 3f_1 + 3f_2 + f_3\right], \quad E_3 = -\frac{3h_3^5}{80} f^{(4)}(\eta), \text{ Simpson's second rule}$$

Newton-Cotes Closed Formulas

$$I_4 : \frac{2h_4}{45}\left[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4\right], \quad E_4 = -\frac{8h_4^7}{945} f^{(6)}(\eta)$$

$$I_5 : \frac{5h_5}{288}\left[19f_0 + 75f_1 + 50f_2 + 50f_3 + 75f_4 + 19f_5\right], \quad E_5 = -\frac{275h_5^7}{12096} f^{(6)}(\eta)$$

$$I_6 : \frac{h_6}{140}\left[41f_0 + 216f_1 + 27f_2 + 272f_3 + 27f_4 + 216f_5 + 41f_6\right],$$

$$E_6 = -\frac{9h_6^9}{1400} f^{(8)}(\eta)$$

Newton-Cotes Closed Formulas

$$I_2 : \frac{h_2}{3}\left[f_0 + 4f_1 + f_2\right], \quad E_2 = -\frac{h^5}{90}f^{(4)}(\eta), \text{ Simpson's first}$$

$$I_3 : \frac{3h_3}{8}\left[f_0 + 3f_1 + 3f_2 + f_3\right], \quad E_3 = -\frac{3h^5}{80}f^{(4)}(\eta), \text{ Simpson's second}$$

- Error for $n = 2$ appears smaller than $n = 3$. Not necessarily true.
- η values are not the same – assume this is not that significant
- h values are not the same!
- $h_2 = (b-a)/2$ and $h_3 = (b-a)/3$ and
- Therefore,

$$E_2 = -\frac{(b-a)^5}{2880}f^{(4)}(\eta_2) \text{ and } E_3 = -\frac{(b-a)^5}{6480}f^{(4)}(\eta_3)$$

Newton-Cotes Open Formulas

- $n + 1$ points in (a, b) with $x_0 = a + h_n$ and $x_n = b - h_n$
- equally spaced points, $x_i = a + (i + 1)h_n, \;\; 0 \leq i \leq n$, i.e., $h_n = (b - a)/(n + 2)$.
- coefficients depend only on n and h_n, i.e., precomputable
- degree of exactness is n when n is odd
- degree of exactness is $n + 1$ when n is even, $\therefore$ odd number of points used typically
- note negative values appear with small n (stability concerns)
- note form of error bound

Newton-Cotes Open Formulas

Be careful with n and h_n definitions when comparing to earlier formulas.

$$I_0 : 2h_0\left[f_0\right], \quad E_0 = \frac{h_0^3}{3} f^{(2)}(\eta), \text{ midpoint rule}$$

$$I_1 : \frac{3h_1}{2}\left[f_0 + f_1\right], \quad E_1 = \frac{3h_1^3}{4} f^{(2)}(\eta)$$

$$I_2 : \frac{4h_2}{3}\left[2f_0 - f_1 + 2f_2\right], \quad E_2 = \frac{14h_2^5}{45} f^{(4)}(\eta)$$

$$I_3 : \frac{5h_3}{24}\left[11f_0 + f_1 + f_2 + 11f_3\right], \quad E_3 = \frac{95h_3^5}{144} f^{(4)}(\eta)$$

$$I_4 : \frac{3h_4}{10}\left[11f_0 - 14f_1 + 26f_2 - 14f_3 + 11f_4\right], \quad E_4 = \frac{41h_4^7}{140} f^{(6)}(\eta)$$

Example

$$I = \int_0^1 e^x dx = 1.718281828\ldots, \quad I_0 = 1.648721271\ldots$$

$$I_1 = 1.859140914\ldots, \quad I_2 = 1.718861152\ldots$$

$$|I - I_0| = 0.069\ldots, \ \ |I - I_1| = 0.1408\ldots, \ \ |I - I_2| = 0.00058\ldots$$

$$h_0 = 0.5, \quad h_1 = 1.0, h_2 = 0.5$$

$$E_0 = \frac{h_0^3}{3} f^{(2)}(\eta_0) \to 0.0416 \approx \frac{1}{24} \leq |E_0| \leq \frac{e}{24} \approx 0.11$$

$$E_1 = -\frac{h_1^3}{12} f^{(2)}(\eta_1) \to 0.083 \approx \frac{1}{12} \leq |E_1| \leq \frac{e}{12} \approx 0.2265$$

$$E_2 = -\frac{h_2^5}{90} f^{(4)}(\eta_2) \to 0.00035 \approx (\frac{1}{2})^5 \frac{1}{90} \leq |E_1| \leq (\frac{e}{2})^5 \frac{1}{90} \approx 0.00094$$

Analysis of Methods

There are multiple analysis methods to determine

- degree of exactness
- order of infinitesimal
- form of the error.

We can exploit polynomial interpolant knowledge or analyze it without such assumptions.

Degree of Exactness in Trapezoidal Rule

Substitute $f = x^k$ into $I_1(f)$ and $I(f)$ and compare for various k.

$$
\begin{aligned}
I(x^k) = \int_a^b x^k &= \frac{1}{k+1}\left(b^{k+1} - a^{k+1}\right) \\
I_1(x^k) &= \frac{(b-a)}{2}\left(a^k + b^k\right) \\
&= \frac{1}{2}\left(b^{k+1} - a^{k+1} + ba^k - ab^k\right) \\
k \le 1 &\rightarrow I(x^k) = I_1(x^k) \\
k > 1 &\rightarrow I(x^k) \neq I_1(x^k)
\end{aligned}
$$

degree of exactness is 1.

Discrete Mean Value Theorem

Theorem 17.2. *If $f(x) \in \mathcal{C}[a,b]$, x_i, $0 \leq i \leq s$ are points in $[a,b]$, and δ_i are scalars with constant sign on $[a,b]$ then*

$$\exists \eta \in [a,b], \quad \sum_{i=0}^{s} \delta_i f(x_i) = f(\eta) \sum_{i=0}^{s} \delta_i$$

Integral Mean Value Theorem

Theorem 17.3. *If $f(x) \in \mathcal{C}[a,b]$ and $g(x) \in \mathcal{C}[a,b]$ and $g(x)$ has constant sign, i.e., $g(x) \geq 0$ or $g(x) \leq 0$ on $a < x < b$ then*

$$\int_a^b g(x)f(x)dx = f(\eta)\int_a^b g(x)dx$$

$$f(\eta) = \frac{\int_a^b g(x)f(x)dx}{\int_a^b g(x)dx}$$

where $a < \eta < b$.

Error in Quadrature

- If the method is an Interpolatory Quadrature method then

$$E_n(f) = I(f) - I_n(f) = \in_a^b (f(x) - p_n(x))dx$$

  and exploit knowledge about form of interpolation error

- If the method is given without any indication of derivation, e.g.,

$$I_n(f) = h \sum_{i=0}^{n} \alpha_i f(x_i)$$

  then use expansions of $f(x_i)$ in both $I_n(f)$ and $I(f)$.

- Examples of the first Trapezoidal Rule and Midpoint Rule
- Example of second Trapezoidal Rule and Simpson's Rule
- See proof of Theorem 9.2 in textbook for another more general approach due to Isaacson and Keller.

Error in Trapezoidal Rule

Use interpolant form of error and IMV Theorem.

$$f(x) \in \mathcal{C}^{(2)}[a,b], \quad h = b-a, \quad x = a+sh, \quad dx = hds$$

$$E_1(f) = \int_a^b f[a,b,x](x-a)(x-b)dx$$

$$= f[a,b,\eta]\int_a^b \big[(x-a)(x-b)\big]dx = \frac{1}{2}h^3 f''(\mu)\int_0^1 s(s-1)ds$$

$$= \frac{1}{2}h^3 f''(\mu)\left[\frac{s^3}{3} - \frac{s^2}{2}\right]_0^1 = -\frac{1}{12}f''(\mu)(b-a)^3$$

Degree of exactness is 1. Order of infinitesimal is 3. Error form required is produced. See Isaacson and Keller Chap. 6.1 for the continuity properties of divided differences even with repeated points (and therefore of $f''(\eta(x))$ w.r.t. x).

Error in Midpoint Rule

Recall Newton-Cotes methods come in pairs with respect to order of error. Midpoint is one that is higher order than expected. Use interpolation error, Taylor expansion (Div. Diff. form) and IMV Theorem.

$f(x) \in \mathcal{C}^{(2)}[a,b], \quad h = \frac{b-a}{2}, \quad x_0 = a + h = b - h$

$$I(f) - I_0(f) = \int_a^b (f(x) - f(x_0))\, dx = \int_a^b (f[x_0, x](x - x_0))\, dx$$

MVT does not apply to second term so expand one more term

$$I(f) - I_0(f) = \int_a^b \left(f[x_0, x_0](x - x_0) + f[x_0, x_0, x](x - x_0)^2\right) dx$$

$$= \frac{f'(x_0)}{2} \left[(x - x_0)^2\right]_a^b + \int_a^b f[x_0, x_0, x](x - x_0)^2 dx$$

Error in Midpoint Rule

As noted before $f[x_0, \ldots, x_n,\ x]$ is continuously differentiable. (therefore so is $f''(\eta(x))$ w.r.t. x. $h = (b-a)/2, \quad x = a + sh, \quad dx = hds$

$$E_0(f) = \frac{f'(x_0)}{2}\left[(x-x_0)^2\right]_a^b + \int_a^b f[x_0, x_0, x](x-x_0)^2 dx$$

$$= \int_a^b f[x_0, x_0, x](x-x_0)^2 dx = f[x_0, x_0, \eta] \int_a^b (x-x_0)^2 dx$$

$$= h\ f[x_0, x_0, \eta] \int_0^2 (a + sh - a - h)^2 ds = h^3\ f[x_0, x_0, \eta] \int_0^2 (s-1)^2 ds$$

$$= h^3\ f[x_0, x_0, \eta]\left[\frac{(s-1)^3}{3}\right]_0^2 = h^3\ f[x_0, x_0, \eta]\left[\frac{1}{3} + \frac{1}{3}\right] = \frac{2}{3} h^3\ f[x_0, x_0, \eta]$$

$$= \frac{1}{3} h^3 f''(\mu) \text{ d.o.e. is } 1\text{, order is } 3$$

Error in Trapezoidal Rule

Suppose we do not assume anything about the interpolant degree or form and simply attempt to use Taylor expansion and the IMV Theorem (and related theorems). We add the assumption that f''' exists.

$$\begin{aligned}
I(f) &= \int_a^b \left[f(a) + (x-a)f'(a) + f''(\eta(x))\frac{(x-a)^2}{2}\right]dx \\
&= hf(a) + \frac{f'(a)}{2}h^2 + \int_a^b f''(\eta(x))\frac{(x-a)^2}{2}dx \\
&= hf(a) + \frac{f'(a)}{2}h^2 + f''(\mu)\int_a^b \frac{(x-a)^2}{2}dx \\
&= hf(a) + \frac{f'(a)}{2}h^2 + \frac{f''(\mu)}{6}h^3
\end{aligned}$$

Error in Trapezoidal Rule

$$I_1(f) = \frac{h}{2}\big[f(a) + f(b)\big]$$

$$= \frac{h}{2}\Big[f(a) + f(a) + hf'(a) + \frac{h^2}{2}f''(\gamma(b))\Big]$$

$$= hf(a) + \frac{f'(a)}{2}h^2 + \frac{f''(\xi)}{4}h^3$$

$$I(f) - I_1(f) = \frac{f''(\mu)}{6}h^3 - \frac{f''(\xi)}{4}h^3$$

Error in Trapezoidal Rule

The discrete mean value theorem does not apply since the coefficients have different signs. So we apply Taylor again to get:

$$
\begin{aligned}
I(f) - I_1(f) &= \frac{h^3}{6} f''(\mu) - \frac{h^3}{4} f''(\xi) \\
&= \frac{h^3}{6} f''(\mu) - \frac{h^3}{4} \left(f''(\mu) + (\xi - \mu) f'''(\zeta)\right) \\
&= -\frac{h^3}{12} f''(\mu) - \frac{h^3}{4} (\xi - \mu) f'''(\zeta) = -\frac{h^3}{12} f''(\mu) + O(h^4)
\end{aligned}
$$

- degree of exactness of 1 follows
- order of infinitesimal of 3 follows
- error coefficient with correct sign found
- not the exact form we had, but good for all practical purposes

Simpson's Rule Error

- $x = x_1 + sh$, $-1 \leq s \leq 1$.
- Apply Taylor expansions around x_1, in $I(f)$ and $I_2(f)$.
- Compute $E_2(f) = I(f) - I_2(f)$

$$f_0 = f_1 - hf_1' + \frac{h^2}{2} f_1'' - \frac{h^3}{3!} f_1''' + \frac{h^4}{4!} f_1'''' + O(h^5)$$
$$f_2 = f_1 + hf_1' + \frac{h^2}{2} f_1'' + \frac{h^3}{3!} f_1''' + \frac{h^4}{4!} f_1'''' + O(h^5)$$

Simpson's Rule Error

$$
\begin{aligned}
\int_a^b f(x)dx &= \int_a^b \{f_1 + (x-x_1)f_1' + \frac{(x-x_1)^2}{2} f_1'' \\
&+ \frac{(x-x_1)^3}{3!} f_1''' + \frac{(x-x_1)^4}{4!} f_1'''' + O((x-x_1)^5) dx\} \\
&= h \int_{-1}^{1} \{f_1 + s f_1' + \frac{s^2 h^2}{2} f_1'' + \frac{s^3 h^3}{3!} f_1''' + \frac{s^4 h^4}{4!} f_1'''' + O(s^5) ds\} \\
&= h f_1 \left[s\right]_{-1}^{1} + \frac{h}{2} f_1' \left[s^2\right]_{-1}^{1} + \frac{h^3}{6} f_1'' \left[s^3\right]_{-1}^{1} + \frac{h^4}{24} f_1''' \left[s^4\right]_{-1}^{1} \\
&+ \frac{h^5}{120} f_1'''' \left[s^5\right]_{-1}^{1} + O(h^6) \\
&= 2h f_1 + \frac{h^3}{3} f_1'' + \frac{h^5}{60} f_1'''' + O(h^6)
\end{aligned}
$$

Simpson's Rule Error

$$f_0 = f_1 - hf_1' + \frac{h^2}{2}f_1'' - \frac{h^3}{3!}f_1''' + \frac{h^4}{4!}f_1'''' - \frac{h^5}{5!}f_1^{(5)} + O(h^6)$$

$$f_2 = f_1 + hf_1' + \frac{h^2}{2}f_1'' + \frac{h^3}{3!}f_1''' + \frac{h^4}{4!}f_1'''' + \frac{h^5}{5!}f_1^{(5)} + O(h^6)$$

$$I_2(f) = \frac{h}{3}(f_0 + 4f_1 + f_2)$$

$$= \frac{h}{3}\{6f_1 + h^2 f_1'' + \frac{2}{4!}h^4 f_1''''\} + O(h^6)$$

Simpson's Rule Error

$$I_2(f) = \frac{h}{3}\{6f_1 + h^2 f_1'' + \frac{2}{4!}h^4 f_1''''\} + O(h^6)$$

$$I(f) = 2hf_1 + \frac{h^3}{3}f_1'' + \frac{h^5}{60}f_1'''' + O(h^6)$$

$$E_2(f) = \{\frac{1}{60} - \frac{1}{36}\}h^5 f_1'''' + O(h^6) = -\frac{1}{90}h^5 f_1'''' + O(h^6)$$

Order of the infinitesmal is 5. The structure of the $O(h^6)$ yields a degree of exactness of 3. A more complicated analysis yields the exact error form:

$$E_2(f) = -\frac{1}{90}h^5 f''''(\eta)$$

e.g., apply proof technique in text for Theorem 9.2 to Simpson's Rule

Newton-Cotes Error

Theorem 17.4. *(Text Thm 9.2 part 1) For any Newton-Cotes formula with n even (odd number of points), the error has the form*

$$E_n(f) = \frac{M_n}{(n+2)!} h^{n+3} f^{(n+2)}(\eta)$$

for $f \in \mathcal{C}^{(n+2)}[a,b]$ and $a < \eta < b$ with

$$M_n = \begin{cases} \int_0^n t\ \pi_{n+1}(t)dt < 0 & \textit{for closed formulas} \\ \int_{-1}^{n+1} t\ \pi_{n+1}(t)dt > 0 & \textit{for open formulas} \end{cases}$$

and $\pi_{n+1}(t) = \prod_{i=0}^{n}(t-i)$. Note h depends on open vs. closed and n.

Newton-Cotes Error

Theorem 17.5. *(Text Thm 9.2 part 2) For any Newton-Cotes formula with n odd (even number of points), the error has the form*

$$E_n(f) = \frac{K_n}{(n+1)!} h^{n+2} f^{(n+1)}(\eta)$$

for $f \in \mathcal{C}^{(n+1)}[a,b]$ and $a < \eta < b$ with

$$K_n = \begin{cases} \int_0^n \pi_{n+1}(t)dt < 0 & \textit{for closed formulas} \\ \int_{-1}^{n+1} \pi_{n+1}(t)dt > 0 & \textit{for open formulas} \end{cases}$$

and $\pi_{n+1}(t) = \prod_{i=0}^{n}(t-i)$. Note h depends on open vs. closed and n.

Design via Moment Matching

- Taylor series can also be used to determine the coefficients of a quadrature method.
- Choose mesh and parameterization.
- Examine the Taylor expansions of $\int_a^b f(x)dx$ and the quadrature method.
- Determine the set of equations that result from setting the coeffients of the terms with matching derivatives equal.
- The first term that cannot be made to match generates the error.
- Solve the equations for the parameters of the method and the error coefficient.

Design Simpson's First Rule

$$h = (b-a)/2, \quad x_i = a + ih, \quad n = 2 \ \ (n+1 \text{ points})$$

$$I(f) = \int_a^b f(x)dx = 2hf_1 + \frac{h^3}{3}f_1'' + \frac{h^5}{60}f_1'''' + O(h^6)$$

$$I_2(f) = h\left(\alpha_0 f_0 + \alpha_1 f_1 + \alpha_2 f_2\right)$$

$$f_0 = f_1 - hf_1' + \frac{h^2}{2}f_1'' - \frac{h^3}{3!}f_1''' + \frac{h^4}{4!}f_1'''' - \frac{h^5}{5!}f_1^{(5)} + O(h^6)$$
$$f_2 = f_1 + hf_1' + \frac{h^2}{2}f_1'' + \frac{h^3}{3!}f_1''' + \frac{h^4}{4!}f_1'''' + \frac{h^5}{5!}f_1^{(5)} + O(h^6)$$

Design Simpson's First Rule

Setting first three coefficients equal yields:

$$2hf_1 = hf_1(\alpha_0 + \alpha_1 + \alpha_2)$$

$$0 = h^2 f_1'(\alpha_2 - \alpha_0)$$

$$\frac{h^3}{3} f_1'' = \frac{h^3}{2} f_1''(\alpha_0 + \alpha_2)$$

Design Simpson's First Rule

The fourth coeffients yield

$$0 = \frac{h^4}{3!} f_1^{(3)} (\alpha_2 - \alpha_0)$$

and is satisfied automatically due to the second coeffient equation.

The fifth coefficents and the asymptotic terms yield the error

$$\left(\frac{1}{60} - \frac{(\alpha_0 + \alpha_2)}{4!} \right) \; h^5 \; f_1^{(4)} + O(h^6)$$

Design Simpson's First Rule

$$\begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 0 \\ \frac{1}{3} \end{pmatrix}$$

nonsingular matrix $\therefore$ unique solution $\begin{pmatrix} \frac{1}{3} \\ \frac{4}{3} \\ \frac{1}{3} \end{pmatrix}$

$$\left(\frac{1}{60} - \frac{(\alpha_0 + \alpha_2)}{4!} \right) \; h^5 \; f_1^{(4)} + O(h^6) = -\frac{1}{90} \; h^5 \; f_1^{(4)} + O(h^6)$$

Peano Error Representation

Theorem 17.6. *Let*

$$N(f) = \sum_{k=0}^{m_0} \alpha_{k,0} f(x_{k,0}) + \sum_{k=0}^{m_1} \alpha_{k,1} f'(x_{k,1}) + \cdots + \sum_{k=0}^{m_\ell} \alpha_{k,\ell} f^{(\ell)}(x_{k,\ell})$$

be a numerical quadrature scheme with degree of exactness n. For all $f(x) \in \mathcal{C}^{(n+1)}[a,b]$ the error in the quadrature is:

$$E(f) = N(f) - I(f) = \int_a^b f^{(n+1)}(t) K(t) dt$$

$$K(t) = \frac{1}{n!} E_x \left[(x-t)_+^n \right], \quad (x-t)_+^n = \begin{cases} (x-t)^n & \textit{if } x \geq t \\ 0 & \textit{if } x < t \end{cases}$$

and $E_x \left[(x-t)_+^n \right]$ is the quadrature error when viewing $(x-t)_+^n$ as a function of x.

Peano Error Representation

See Stoer and Bulirsch textbook for a detailed discussion.

Simpson's Rule has degree of exactness $n = 3$ and the Peano kernel $K(t)$ on $[-1, 1]$ is

$$K(t) = \frac{1}{6}\Big[\frac{1}{3}(-1-t)_+^3 + \frac{4}{3}(0-t)_+^3 + \frac{1}{3}(1-t)_+^3 - \int_{-1}^{1}(x-t)_+^3\,dx\Big]$$
$$= \begin{cases} \frac{1}{72}(1-t)^3(1+3t) & \text{if } 0 \le t \le 1 \\ K(-t) & \text{if } -1 \le t \le 0 \end{cases}$$

Note. For Simpson's Rule, $K(t)$ has constant sign.

Peano Error Representation

Corollary 17.7. *If the Peano kernel $K(t)$ has constant sign on $[a,b]$ then*

$$\exists \eta \in [a,b], \quad E(f) = N(f) - I(f) = \int_a^b f^{(n+1)}(t)K(t)dt$$
$$= f^{(n+1)}(\eta) \int_a^b K(t)dt$$

Corollary 17.8. *The Peano kernel $K(t)$ has constant sign on $[a,b]$ for all of the Newton-Cotes quadrature formulas.*

The Peano Theorem holds for all quadrature methods where the operators E and E_x commute with integration.

Peano Kernel Derivation of Error

Consider Simpson's First Rule with degree of exactness $n = 3$ on $[-1, 1]$.
$\therefore h = 1$.

$$-1 \le t \le 1, \quad \frac{1}{3}(-1 - t)_+^3 = 0$$

$$-1 \le t \le 1, \quad \frac{1}{3}(1 - t)_+^3 = \frac{1}{3}(1 - t)^3$$

$$\frac{4}{3}(0 - t)_+^3 = \begin{cases} 0 & \text{if } 0 \le t \le 1 \\ -\frac{4}{3}t^3 & \text{if } -1 \le t \le 0 \end{cases}$$

Peano Kernel Derivation of Error

$$\int_{-1}^{1}(x-t)_+^3\,dx = \int_t^1 (x-t)^3\,dx = \int_0^{(1-t)} s^3\,ds = \frac{1}{4}(1-t)^4$$

$$6\mathcal{K}(t) = \frac{1}{3}(-1-t)_+^3 + \frac{4}{3}(0-t)_+^3 + \frac{1}{3}(1-t)_+^3 - \int_{-1}^{1}(x-t)_+^3\,dx$$

$$6\mathcal{K}(t) = \frac{1}{3}(1-t)^3 - \frac{1}{4}(1-t)^4 + g(t) = \frac{1}{12}(1-t)^3(1+3t) + g(t)$$

$$g(t) = \begin{cases} 0 & \text{if } 0 \le t \le 1 \\ -\frac{4}{3}t^3 & \text{if } -1 \le t \le 0 \end{cases}$$

Peano Kernel Derivation of Error

Let $r = |t|$ and note

$$p(t) = \frac{1}{3}(1-t)^3 - \frac{1}{4}(1-t)^4 = -\frac{1}{4}t^4 + \frac{2}{3}t^3 - \frac{1}{2}t^2 + \frac{1}{12}$$

$$p(t) = \begin{cases} -\frac{1}{4}r^4 + \frac{2}{3}r^3 - \frac{1}{2}r^2 + \frac{1}{12} & \text{if } 0 \le t \le 1 \\ -\frac{1}{4}r^4 - \frac{2}{3}r^3 - \frac{1}{2}r^2 + \frac{1}{12} & \text{if } -1 \le t \le 0 \end{cases}$$

$$\therefore -1 \le t \le 0, \;\; p(t) = p(r) + \frac{4}{3}t^3 = p(-t) + \frac{4}{3}t^3$$

$$-1 \le t \le 0, \;\; 6\mathcal{K}(t) = p(t) - \frac{4}{3}t^3 = p(-t) = 6\mathcal{K}(-t) \qquad \Box$$

Peano Kernel Derivation of Error

We know from earlier analysis that

$$I(f) - I_2(f) = -\frac{h^5}{90} f^{(4)}(\eta)$$

For $[-1, 1]$, $h = 1$ and the Peano Kernel Error Theorem says

$$I_2(f) - I(f) = f^{(4)}(\eta) \int_{-1}^{1} \mathcal{K}(t)dt$$

$$= \frac{f^{(4)}(\eta)}{6} \times 2 \int_0^1 p(t)dt = \frac{f^{(4)}(\eta)}{3} \times \frac{8}{40} \frac{f^{(4)}(\eta)}{90} \text{ by symmetry}$$

or by definition

$$\frac{f^{(4)}(\eta)}{6} \left[\int_{-1}^{1} p(t)dt - \frac{4}{3} \int_{-1}^{0} t^3 dt \right] = \frac{f^{(4)}(\eta)}{6} \left[-\frac{32}{120} + \frac{40}{120} \right] = \frac{f^{(4)}(\eta)}{90}$$

Newton-Cotes Composite Formulas

- When $b - a$ is large or n is too large to trust a Newton-Cotes formula, composite N-C formulas can be used.
- f is approximated by a piecewise interpolant
- N-C formula is used on each piece.
- open or closed formula may be used.
- Error can be reduced by adding more intervals.
- order of infinitesimal determines the rate of convergence of $E(f) = I(f) - I_n(f)$.
- As with piecewise interpolation, the size of each interval can be tuned based on knowledge of the appropriate derivative of $f(x)$ to guarantee a desired accuracy.

Composite Trapezoidal Rule

We have

$$a = x_0 < x_1 < \cdots < x_n = b$$

$$h = \frac{b-a}{n} \text{ and } x_{i+1} = x_i + h,\ 0 \le i \le n-1$$

$$I_i = \frac{h}{2}(f(x_{i+1}) + f(x_i)) \text{ and } I_n(f) = \sum_{i=0}^{n-1} I_i$$

$$I_n(f) = \frac{h}{2}(f_0 + f_n) + h\sum_{i=1}^{n-1} f_i = \frac{h}{2}\left[f_0 + f_n + 2\sum_{i=1}^{n-1} f_i\right]$$

Composite Trapezoidal Rule

We have $h = (b-a)/n$ and the error

$$E_i = -\frac{h^3}{12} f''(\eta_i) \to E = -\frac{h^3}{12} \sum_{i=0}^{n-1} f''(\eta_i)$$

$$= -\frac{h^3}{12} n f''(\mu) = -\frac{h^2}{12}(b-a) f''(\mu)$$

since by the Discrete Mean Value Theorem

$$\exists \mu \ni f''(\mu) = \frac{1}{n} \sum_{i=0}^{n-1} f''(\eta_i)$$

Composite Newton-Cotes Error

Given m intervals in $[a, b]$, on each of which a Newton-Cotes quadrature formula is used with errors E_i, $0 \leq i \leq m$ we have a total error of

$$E = \sum_{i=1}^{m} E_i$$

where E_i depends on the method and the value of n where $n + 1$ points are used within each interval.

Composite Newton-Cotes Error

Theorem 17.9. *If m intervals of size H are used with a Newton-Cotes method on each with $n+1$ points then*

$$E_{n,m}(f) = \begin{cases} C_{n,m} H_m^{n+2} f^{(n+2)}(\mu) & \textit{if } n \textit{ is even} \\ \tilde{C}_{n,m} H_m^{n+1} f^{(n+1)}(\mu) & \textit{if } n \textit{ is odd} \end{cases}$$

- Text Theorem 9.3 gives the details of the constants which depend on if the Newton-Cotes method is open or closed.
- n even has degree of exactness of $n+1$ and order of infinitesimal of $n+2$
- n odd has degree of exactness of n and order of infinitesimal of $n+1$
- $h = H/n$ (closed) and $h = H/(n+2)$ (open) are the subinterval sizes use in each Newton-Cotes method application