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Section 5.2: Error in T_n and S_n[1]

Consider the partiaion $a = x_0 < x_1 < \cdots < x_n = b$ of equally spaced nodes with $h = x_{j+1} - x_j$. On the subinterval $[x_j, x_{j+1}]$ we have the error formula for P_1 (assuming f'' exists)

$$f(x) - P_1(x) = \frac{(x - x_j)(x - x_{j+1})}{2} f''(c_j) \quad \text{for some} \quad x_j \le c_j \le x_{j+1}.$$

[1] We consider only the case of an equally spaced partition.

Error Formula for T_n (one subinterval)

Compute the integral.

$$\int_{x_j}^{x_{j+1}} \frac{(x-x_j)(x-x_{j+1})}{2}\,dx = \frac{1}{2}\int_0^h u(u-h)\,du \quad \text{where} \quad u = x - x_j$$

$u = x - x_j, \quad du = dx, \quad x - x_{j+1} = u + x_j - x_{j+1}$

$= u - \underbrace{(x_{j+1} - x_j)}_{h} = u - h$

when $x = x_j, \; u = x_j - x_j = 0$

$x = x_{j+1}, \; u = x_{j+1} - x_j = h$

$$\frac{1}{2}\int_0^h u(u-h)\,du = \frac{1}{2}\int_0^h (u^2 - uh)\,du$$

$$= \frac{1}{2}\left[\frac{u^3}{3} - \frac{u^2}{2}h\right|_0^h$$

$$= \frac{1}{2}\left[\frac{h^3}{3} - \frac{h^2}{2}\cdot h - 0\right] = \frac{1}{2}\left[\frac{h^3}{3} - \frac{h^3}{2}\right]$$

$$= \frac{1}{2}\left(\frac{-h^3}{6}\right) = \frac{-h^3}{12}$$

Error Formula for T_n (over whole subinterval)

From the previous integral, the error over just the subinterval $[x_j, x_{j+1}]$ is found to be

$$\begin{aligned}
\text{Error} &= \int_{x_j}^{x_{j+1}} f(x)\,dx - \int_{x_j}^{x_{j+1}} P_1(x)\,dx \\
&= \int_{x_j}^{x_{j+1}} (f(x) - P_1(x))\,dx \\
&= -\frac{h^3}{12} f''(c_j)
\end{aligned}$$

For some number $x_j < c_j < x_{j+1}$.

To get the error over the whole interval $[a, b]$, we use the additive property of integrals and sum

$$-\frac{h^3}{12} f''(c_0) - \frac{h^3}{12} f''(c_1) - \cdots - \frac{h^3}{12} f''(c_{n-1})$$

Error E_n^T Formula for T_n

Writing

$$\frac{h^3}{12} = \left(\frac{h^2}{12}\right)\ h$$

we can add the errors from $[x_0, x_1]$, $[x_1, x_2]$, etc. together to get

$$E_n^T(f) = -\frac{h^2}{12}\left[hf''(c_0) + hf''(c_1) + \cdots + hf''(c_{n-1})\right]$$

If we set $h = \Delta x$, then the bracketed expression is

$$f''(c_0)\Delta x + f''(c_1)\Delta x + \ldots + f''(c_{n-1})\Delta x$$

$$= \sum_{i=0}^{n-1} f''(c_i)\,\Delta x$$

We're using E for error with a superscript T for the rule and subscript n for the number of subintervals.

Error E_n^T Formula for T_n

Recognizing the expression in brackets [ ] as a Riemann sum, we have

$$E_n^T(f) = -\frac{h^2}{12}\left[hf''(c_0) + hf''(c_1) + \cdots + hf''(c_{n-1})\right]$$

$$\approx -\frac{h^2}{12}\int_a^b f''(x)dx = \frac{-h^2}{12}\left[f'(x) \Big|_a^b \right.$$

$$= \frac{-h^2}{12}\left(f'(b) - f'(a) \right)$$

By the Mean Value Theorem

$$f'(b) - f'(a) = (b-a)f''(c), \quad \text{for some} \quad a \le c \le b.$$

Error E_n^T Formula for T_n

Our final error formula is

$$E_n^T(f) = I(f) - T_n(f) = -\frac{h^2}{12}(b-a)f''(c)$$

for some c between a and b.

Since $h = (b-a)/n$, we can express E_n^T in terms of n as

$$E_n^T(f) = -\frac{(b-a)^3}{12n^2}f''(c).$$

We see that the error is proportional to $\frac{1}{n^2}$.

Example

Estimate the number of subintervals needed to guarantee an accuracy

$$|E_n^T(f)| \le 10^{-4}$$

for the integral

$$I(f) = \int_0^1 \frac{dx}{1+x}.$$

$$|E_n^T(f)| = \left| \frac{-(b-a)^3}{12n^2} \cdot f''(c) \right|$$ for some c between a and b.

$b = 1, \quad a = 0 \qquad f(x) = \frac{1}{1+x}, \quad f'(x) = \frac{-1}{(1+x)^2}, \quad f''(x) = \frac{2}{(1+x)^3}$

f'' is decreasing so $\quad |f''(c)| \le |f''(0)| = \frac{2}{(1)^3} = 2$

So $\left|E_n^T(f)\right| \le \frac{1^3}{12n^2}\cdot 2 = \frac{1}{6n^2}$, we need $\frac{1}{6n^2} \le 10^{-4}$

This requires $n^2 \geq \frac{1}{6\cdot 10^{-4}} = \frac{10^4}{6} = \frac{5000}{3}$

$$n \geq \sqrt{\frac{5000}{3}} \approx 40.82$$

So $n = 41$ will guarentee the desired accuracy.

Error in Trapezoid Rule

$$I(f) = \int_0^1 \frac{dx}{x+1} = \ln 2 \doteq 0.693147181$$

n	T_n	E_n^T	$(E_n^T)/(E_{2n}^T)$
2	0.70833333	-0.01518615	3.9174
4	0.69702381	-0.00387663	3.9774
8	0.69412185	-0.00097467	3.9942
16	0.693391202	-0.00024402	

Since $E_n^T \propto \frac{1}{n^2}$, doubling the number of subintervals reduces the error by a factor of 4.

Error in Simpson's Rule E_n^S

A similar derivation shows that for f sufficiently differentiable,

$$E_n^S(f) = I(f) - S_n(f) = -\frac{h^4}{180}(b-a)f^{(4)}(c)$$

for some c between a and b. Since $h = (b-a)/n$, the above can be written as

$$E_n^S(f) = -\frac{(b-a)^5}{180n^4}f^{(4)}(c)$$

Note that the payoff for using the more complicated Simpson's rule is that the error is proportional to $\frac{1}{n^4}$.

Example

Estimate the number of subintervals needed[2] to guarantee an accuracy

$$|E_n^S(f)| \leq 10^{-4}$$

for the integral

$$I(f) = \int_0^1 \frac{dx}{1+x}.$$

$$|E_n^S(f)| = \left| \frac{-(b-a)^5}{180\, n^4} f^{(4)}(c) \right| , \quad f''(x) = \frac{2}{(1+x)^3} , \quad f'''(x) = \frac{-6}{(1+x)^4}$$

$$f^{(4)}(x) = \frac{24}{(1+x)^5}$$

so $\left| f^{(4)}(c) \right| \leq \left| f^{(4)}(0) \right| = 24$

[2]Recall that n must be even!

$$\left|E_n^S(f)\right| \le \frac{1^5}{180n^4}\cdot 24 = \frac{2}{15n^4}$$, we want this $\le 10^{-4}$

$$\frac{2}{15n^4} \le 10^{-4} \Rightarrow n^4 \geq \frac{2}{15\cdot 10^{-4}} = \frac{2\cdot 10^4}{15} = \frac{4000}{3}$$

$$n \geq \sqrt[4]{\frac{4000}{3}} \approx 6.04$$

Since n must be even, taking $n=8$ will give the desired accuracy.

Error in Simpson's Rule

$$I(f) = \int_0^1 \frac{dx}{x+1} = \ln 2$$

n	S_n	E_n^S	$(E_n^S)/(E_{2n}^S)$
2	0.69444444	-0.00129726	12.148
4	0.69325397	-0.00010679	14.529
8	0.69315453	-0.00000735	15.638
16	0.69314765	-0.00000047	

Since $E_n^S \propto \frac{1}{n^4}$, doubling the number of subintervals reduces the error by up to a factor of 16.

Order of a Rule

Note that the errors have the form

$$\text{Error} \approx \frac{c}{n^p}$$

for some numbers p and c. In particular

$$E_n^T(f) = \frac{c}{n^2}, \quad \text{and} \quad E_n^S(f) = \frac{c}{n^4}$$

for many functions f.

We may refer to p as the **order** of the integration rule.

So T is order 2 and S is order 4.

Richardson Extrapolation

Let an integration rule be denoted by I_n and have order p. The Richardson extrapolation formula for this integration rule is

$$R_{2n} = \frac{1}{2^p - 1}\left(2^p I_{2n} - I_n\right).$$

In particular, for the Trapezoid rule

$$R_{2n} = \frac{1}{3}\left(4T_{2n} - T_n\right).$$

In particular, for Simpson's rule

$$R_{2n} = \frac{1}{15}\left(16S_{2n} - S_n\right).$$

Richardson Extrapolation

The Richardson extrapolation formula for integration rule I_n of order p is

$$R_{2n} = \frac{1}{2^p - 1}\left(2^p I_{2n} - I_n\right).$$

Note: If you're computing I_{2n}, then you've already found all of the necessary information to compute I_n. Then computing R_{2n} only requires two multiplications and one subtraction with numbers you've already found!

Example

Use the previous results for the **Trapezoid** rule to compute $R_4(f)$ for

$$\int_0^1 \frac{dx}{x+1}$$

and compare the error of R_4 to that of T_8.

For trapezoid $R_4 = \frac{1}{3}(4T_4 - T_2)$

using the previous table

$$= \frac{1}{3}(4 \cdot 0.69702381 - 0.70833333)$$

$$\doteq 0.69325397\mathrm{0}$$

$$Err(R_4) = \ln 2 - R_4 \doteq -0.00010679$$

$$Rel(R_4) = \frac{Err(R_4)}{\ln 2} \doteq 0.000154$$

$$E_8^T(f) \doteq -0.00097467$$

$$Rel(T_8(f)) \doteq 0.001406$$

R_4 gain is about a factor of 10

Example

Use the previous results for the **Simpson's** rule to compute $R_4(f)$ for

$$\int_0^1 \frac{dx}{x+1}$$

and compare the error of R_4 to that of S_4.

For Simpson's rule $\quad R_4 = \frac{1}{15}\left(16 S_4 - S_2\right)$

$$R_4 = \frac{1}{15}\left(16 \cdot 0.693253970 - 0.694444444\right)$$

$$\doteq 0.693174605$$

$$Err(R_4) = \ln 2 - R_4 \doteq -0.0000274$$

$$Rel(R_4) = \frac{Err(R_4)}{\ln 2} \doteq -0.0000396$$

$$E_4^S(f) = -0.000107$$

$$Rel(S_4(f)) = 0.000154$$

R_4 gain is about a factor of 4

Section 5.3: Gaussian Quadrature

Consider the integral $I(f) = \int_{-1}^{1} f(x)\, dx$ [3]. Both the Trapezoid and Simpson's rule start with approximating f by a polynomial to obtain the rule. Both rules have a certain form.

$$T_n(f) = \frac{h}{2}[f(x_0) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(x_n)]$$

$$= w_0 f(x_0) + w_1 f(x_1) + \cdots + w_{n-1} f(x_{n-1}) + w_n f(x_n)$$

$$= \sum \text{numbers} \cdot \text{function values.}$$

[3] We can consider more general limits $[a, b]$ later.

Gaussian Quadrature

Here we are going to approximate the integral $I(f)$ by the new *rule* called **Gaussian Quadrature**. The integration formula will be given by

$$I_n(f) = \sum_{j=1}^{n} w_j f(x_j)$$

where the numbers $\{w_1, \ldots, w_n\}$ are called the **weights** and $\{x_1, \ldots, x_n\}$ are called the **nodes.**

Main Idea: The weights and nodes are chosen so that $I_n(p) = I(p)$ exactly, for $p(x)$ any polynomial of degree as high as possible.

Gaussian Quadrature: $n = 1$ Case

When $n = 1$, the formula becomes

$$I_1(f) = \sum_{j=1}^{1} w_j f(x_j) = w_1 f(x_1).$$

There is one weight w_1 and one node x_1.

We need to determine two things, w_1 and x_1, so we can impose two conditions. We'll insist that the formula is exact for all polynomials of degree 1—i.e. all polynomials of the form $p(x) = p_0 + p_1 x$.

Building Block of Polynomials

We note that a polynomial

$$p(x) = p_0 + p_1 x + p_2 x^2 + \cdots + p_n x^n$$

is a linear combination (sum of constant multiples of) the basic building blocks

$$1, \quad , x, \quad x^2, \quad \cdots, \quad x^n$$

Because integrating is a *linear transformation*

$$\text{i.e.} \quad \int (\alpha f(x) + \beta g(x))\, dx = \alpha \int f(x)\, dx + \beta \int g(x)\, dx$$

we will use these building blocks to obtain our weights and nodes. [4]

[4] An alternative approach using the theory of orthogonal polynomials can be used (see pg. 223 of our text).

Gaussian Quadrature: $n = 1$ Case

$$\int_{-1}^{1} f(x)\,dx \approx I_n(f) = w_1 f(x_1)$$

The formula should be exact for $p(x) = 1$.

$$\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} 1\,dx = x\Big|_{-1}^{1} = 1-(-1) = 2$$

$$I_1(p) = \int_{-1}^{1} 1\,dx = w_1 p(x_1) = 2 \qquad p(x_1) = 1$$

$$\Rightarrow \quad w_1 \cdot 1 = 2 \quad \text{i.e.} \quad w_1 = 2$$

Gaussian Quadrature: $n = 1$ Case

$$\int_{-1}^{1} f(x)\,dx \approx I_n(f) = w_1 f(x_1)$$

The formula should be exact for $p(x) = x$.

$$\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} x\,dx = \left.\frac{x^2}{2}\right|_{-1}^{1} = \frac{1^2}{2} - \frac{(-1)^2}{2} = 0$$

$$I_1(p) = \int_{-1}^{1} p(x)\,dx = w_1\, p(x_1) = 0 \qquad p(x_1) = x_1$$

$$\Rightarrow \quad 2x_1 = 0 \quad \Rightarrow \quad x_1 = 0$$

Deduce the Guassian Quadrature formula $I_1(f)$

We found that $\int_{-1}^{1} 1\,dx = 2$ and $\int_{-1}^{1} x\,dx = 0$.

Hence $w_1 = 2$ and $x_1 = 0$.

So $I_1(f) = w_1 f(x_1) = 2f(0)$

Gaussian Quadrature: $\int_{-1}^{1} f(x)\,dx \approx I_1(f) = 2f(0)$

Use $I_1(f)$ to approximate $\int_{-1}^{1} \frac{dx}{1+x^2}$. Compare the result to the true value $\frac{\pi}{2}$.

Here $f(x) = \dfrac{1}{1+x^2}$ and $f(0) = \dfrac{1}{1+0^2} = 1$

$$\int_{-1}^{1} \frac{dx}{1+x^2} \approx I_1(f) = 2f(0) = 2\cdot 1 = 2$$

$$\mathrm{Err}(I_1(f)) = \frac{\pi}{2} - 2 \doteq -0.4292$$

Gaussian Quadrature: $n = 2$ Case

When $n = 2$, the formula becomes

$$I_2(f) = \sum_{j=1}^{2} w_j f(x_j) = w_1 f(x_1) + w_2 f(x_2).$$

There are two weights $\{w_1, w_2\}$ and two nodes $\{x_1, x_2\}$.

We have four things to determine, so we can impose four conditions.

Cubics have four conditions $p_0 + p_1 x + p_2 x^2 + p_3 x^3$

Gaussian Quadrature: $n = 2$ Case

We'll insist that the formula is exact for $p(x) = 1, x, x^2$, and x^3.

$$\int_{-1}^{1} 1\,dx = 2 = w_1 + w_2$$

$$\int_{-1}^{1} x\,dx = 0 = w_1x_1 + w_2x_2$$

$$\int_{-1}^{1} x^2\,dx = \frac{2}{3} = w_1x_1^2 + w_2x_2^2$$

$$\int_{-1}^{1} x^3\,dx = 0 = w_1x_1^3 + w_2x_2^3$$

Since x_1 and x_2 are from $[-1, 1]$, we can assume that $-1 \le x_1 < x_2 \le 1$. In fact, since our simple monomials all have symmetry (even or odd), it's safe to assume that x_1 and x_2 will be symmetric about zero.

Gaussian Quadrature: $n = 2$ Case

We have four equations in four unknowns

$$w_1 + w_2 = 2 \quad (1)$$

$$w_1 x_1 + w_2 x_2 = 0 \quad (2)$$

$$w_1 x_1^2 + w_2 x_2^2 = \frac{2}{3} \quad (3)$$

$$w_1 x_1^3 + w_2 x_2^3 = 0 \quad (4)$$

From (2), $w_1 x_1 = -w_2 x_2$ and from (4) $w_1 x_1^3 = -w_2 x_2^3$.

If $w_1 \neq 0$ and $w_2 \neq 0$ we can divide to get

$$\frac{w_1 x_1^3}{w_1 x_1} = \frac{-w_2 x_2^3}{-w_2 x_2} \Rightarrow x_1^2 = x_2^2$$

So $x_1 = -x_2$ or $x_1 = x_2$

Then $w_1 x_1^2 + w_2(-x_1)^2 = \frac{2}{3}$

$(w_1 + w_2)\, x_1^2 = \frac{2}{3}$ but $w_1 + w_2 = 2$

so $x_1^2 = \frac{1}{3} \implies x_1 = \frac{-1}{\sqrt{3}}$ and $x_2 = \frac{1}{\sqrt{3}}$

Also $w_1 x_1 = -w_2 x_2 = -w_2(-x_1)$

$w_1 x_1 = w_2 x_1 \implies w_1 = w_2$

Since $w_1 + w_2 = 2 \Rightarrow 2w_1 = 2 \quad w_1 = w_2 = 1$

The weights are $w_1 = w_2 = 1$

the nodes are

$$x_1 = \frac{-1}{\sqrt{3}}, \quad x_2 = \frac{1}{\sqrt{3}}.$$