MA 668-Numerical Analysis I
Numerical Integration

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Numerical Integration

We want to approximate

$$I_f = \int_a^b f(x)dx \approx \overbrace{\sum_{j=0}^{n} w_j f(x_j)}^{\text{quadrature rule}}$$

- f: integrable
- Abscissae $x_j \in [a, b]$ has weights w_j.

Basic quadrature algorithm

It is based on low degree polynomial. Given $f(x)$, $x \in [a, b]$,

- we choose $x_0, x_1, \cdots, x_n \in [a, b]$
- construct a polynomial interpolant $p_n(x)$
- $\int_a^b f(x)dx \approx \int_a^b p_n(x)dx$

The Lagrange interpolating polynomial:

$$p_n(x) = \sum_{j=0}^{n} f(x_j)L_j(x), \quad L_j(x) = \prod_{\substack{i=0 \\ i\neq j}}^{n} \frac{x - x_i}{x_j - x_i}$$

Therefore, $\int_a^b f(x)dx \approx \int_a^b p_n(x)dx = \sum\limits_{j=0}^{n} f(x_j) \int_a^b L_j(x)dx$, thus

$$w_j = \int_a^b L_j(x)dx.$$

Basic quadrature algorithm

- **Trapezoidal rule**
  - $n = 1;\ \ x_0 = a,\ x_1 = b.$

$$L_0(x) = \frac{x-b}{a-b},\ \ L_1(x) = \frac{x-a}{b-a}$$

$$I_f \approx I_{trap} =$$

- **Simpson rule**
  - $n = 2,\ x_0 = a,\ x_1 = \frac{b+a}{2},\ x_2 = b$

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)},\ L_1(x) = ?,\ L_2(x) = ?$$

$$I_f \approx I_{Simp} = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{b+a}{2}\right) + f(b)\right]$$

Newton-Cotes formulas: Equally spaced points

- **Examples:** Based on polynomial interpolation
  - **Mid point rule**

$$I_f \approx I_{mid} = (b-a)f\left(\frac{a+b}{2}\right)$$

  - Trapezoidal rule
  - Simpson rule
- If the end points a and b are included in $x_0, x_1, \cdots, x_n$, then the formula is **closed**, otherwise, **open Newton-Cotes** formula.

Basic quadrature error

Given $\{(x_i, y_i)\}_{i=0}^n$.

- Interpolation error:

$$f(x) - p_n(x) = f[x_0, x_1, \cdots, x_n, x] \prod_{i=0}^{n} (x - x_i)$$

- Quadrature error:

$$\begin{aligned} E(f) &= \int_a^b f(x)dx - \sum_{j=0}^{n} w_j f(x_j) \\ &= \int_a^b f[x_0, x_1, \cdots, x_n, x] \prod_{i=0}^{n} (x - x_i) dx \end{aligned}$$

Basic quadrature error

- Error in Mid-point rule:

$$E(f) = \frac{f''(\xi)}{24}(b-a)^3$$

- Error in Trapezoidal rule:

$$E(f) = \int_a^b f[a,b,x](x-a)(x-b)dx = -\frac{f''(\xi)}{12}(b-a)^3$$

- Error in Simpson rule:

$$E(f) = \int_a^b f[a, \frac{a+b}{2}, b, x](x-a)\left(x - \frac{a+b}{2}\right)(x-b)dx$$
$$= -\frac{f''''(\xi)}{90}\left(\frac{b-a}{2}\right)^5$$

  - Cost of evaluation is higher

Example 1: $a = 0,\ b = 1,\ f(x) = e^{-x}$

- $I_f = \int_0^1 e^{-x} dx = 1 - \frac{1}{e} \approx 0.63212056$
- $I_{mid} \approx 0.60653066$
- $I_{trap} \approx 0.68393972$
- $I_{simp} \approx 0.63233368$

Example 2: $a = 0.9,\ b = 1,\ f(x) = e^{-x}$

- $I_f = \int_{0.9}^1 e^{-x} dx = \frac{1}{e^{0.9}} - \frac{1}{e} \approx 0.03869021856$
- $I_{mid} \approx 0.03867410234$
- $I_{trap} \approx 0.03872245504$
- $I_{simp} \approx 0.03869021991$

Precision

Precision (also called *degree of accuracy*) of a quadrature formula is the largest integer ρ such that $E(p_n) = 0$ for all polynomials $p_n(x)$ of degree $n \leq \rho$.

- Trapezoidal and mid-point rules have precision 1
- Simpson rule has precision 3

Composite numerical integration

Even for a very smooth integrand the basic quadrature rules may be ineffective when the integration is performed over a long interval.
Remedy

- More sampling of $f(x)$ is intuitively required in such cases.
- Increasing the order of the Newton-Cotes formulas
  - High precision formulas suffer the same problems that high degree polynomial interpolation experiences over long intervals
- Approximating $f(x)$ with piecewise polynomials
  - Resulting quadrature formulas called *composite rules* or **composite quadrature methods**

Composite numerical integration

Consider

$$a = t_0 < t_1 < \cdots < t_{r-1} < t_r = b$$

,

- $t_i = a + ih, \; i = 0, 1, \cdots, r$
- $h = \frac{b-a}{r}$

Then,

$$\int_a^b f(x)dx = \sum_{i=1}^{r} \int_{a+(i-1)h}^{a+ih} f(x)dx = \sum_{i=1}^{r} \int_{t_{i-1}}^{t_i} f(x)dx$$

$E_i(f) = K_i h^{q+1}, \; q \in \mathbb{N}$, then

$$E(f) = \sum_{i=1}^{r} E_i(f) = h^{q+1} \sum_{i=1}^{r} K_i \underbrace{=}_{IVT} h^{q+1} rK = K(b-a)h^q$$

for an appropriate K

Composite trapezoidal method:

$$\int_{t_{i-1}}^{t_i} f(x)dx \approx \frac{h}{2}\left[f(t_i) + f(t_{i-1})\right]$$

Then

$$\int_a^b f(x)dx \approx \frac{h}{2}\sum_{i=1}^{r}\left[f(t_i) + f(t_{i-1})\right]$$

$$\approx \frac{h}{2}[f(a) + 2f(t_1) + 2f(t_2) + \cdots + 2f(t_{r-1}) + f(b)]$$

$$E(f) = \sum_{i-1}^{r}\left(-\frac{f''(\xi_i)}{12}h^3\right) = -\frac{(b-a)h^2}{12}f''(\xi)$$

for some $a \leq \xi \leq b$.

- $O(h^2)$

Composite methods

Composite Simpson method:

- r: even
- $\underbrace{[t_{2k-2}, t_{2k}]}_{2h}$: $k = 1, 2, \cdots, \frac{r}{2}$, double subinterval
- $\int_{t_{2k-2}}^{t_{2k}} f(x)dx \approx \frac{2h}{6}\left[f(t_{2k-2}) + 4f(t_{2k-1}) + f(t_{2k})\right]$
- $\int_a^b f(x)dx \approx \frac{h}{3}\left[f(a) + 2\sum_{k=1}^{\frac{r}{2}-1} f(t_{2k}) + 4\sum_{k=1}^{\frac{r}{2}} f(t_{2k-1}) + f(b)\right]$
- $E(f) = -\frac{f''''(\xi)}{180}(b-a)h^4,\ O(h^4)$

Composite Mid-point method:

- $\int_a^b f(x)dx \approx h\sum_{k=1}^{r} f(a + (k - \frac{1}{2})h)$
- $E(f) = \frac{f''(\xi)}{24}(b-a)h^2,\ O(h^2)$

Example

- $I = \int_0^1 e^{-x^2} dx \approx 0.746824133\cdots,\ h = 0.25$
- $I_{mid} =$
- $I_{trap} =$
- $I_{Simp} =$

Example

Approximate $\int_0^1 e^{-x^2} dx$ with an absolute error less than 10^{-5}. Here $f(x) = e^{-x^2}$

- Composite Simpson method
  - $E(f) = -\frac{f^{''''}(\xi)(b-a)h^4}{180}$
  - $r \geq ?$
  - $I_{simp} = ?$
- Composite Trapezoidal method
  - $E(f) = -\frac{f^{''}(\xi)(b-a)h^2}{12}$
  - $r \geq ?$
  - $I_{simp} = ?$

Note:

- Generally speaking, if the integrand is smooth and the required accuracy is higher, then the higher order methods are more efficient
- For rough integrands, the lower order methods may perform better

$$|E(f)| \leq c\|f^{(q)}\|h^q$$

Quadrature Errors

- Composite trapezoidal method:

$$|E(f)| \leq \frac{\|f^{''}\|_\infty}{12}(b-a)h^2$$

- Composite mid-point method:

$$|E(f)| \leq \frac{\|f^{''}\|_\infty}{24}(b-a)h^2$$

- Composite Simpson method:

$$|E(f)| \leq \frac{\|f^{''''}\|_\infty}{180}(b-a)h^4$$

Gaussian Quadrature

Composite rule of order q has an error:

$$|E(f)| \leq Ch^q \|f^{(q)}\|$$

- $a \leq x_0 < x_1 < \cdots < x_n \leq b$
- $E(f) = \int_a^b (f(x) - p_n(x))dx = \int_a^b f[x_0, x_1, \cdots, x_n, x] \prod_{i=0}^{n} (x - x_i)dx$
- $f[x_0, x_1, \cdots, x_n, x] = \frac{f^{(n+1)}(\xi)}{(n+1)!}$
- If $f(x)$: is a polynomial of degree m, $m > n$, then $f[x_0, x_1, \cdots, x_n, x]$: is a polynomial of degree ?

Zeros of Legendre Polynomials on $[-1, 1]$:

- $\phi_0(x) = 1$
- $\phi_1(x) = x$
- $(j+1)\phi_{j+1}(x) = (2j+1)x\phi_j(x) - j\phi_{j-1}(x), \;\; j \geq 1$
- $\int_{-1}^{1} \phi_i(x)\phi_j(x)dx = 0, \;\; i \neq j$

Note that: For a class of orthogonal polynomials $\phi_0(x), \phi_1(x), \cdots, \phi_{n+1}(x)$ that satisfy

$$\int_a^b \phi_i(x)\phi_j(x)dx = 0, \;\; i \neq j,$$

we have

$$\int_a^b g(x)\phi_{n+1}(x)dx = 0$$

for any polynomial $g(x)$ of degree $\leq n$.

Gaussian Quadrature

Thus, we choose the points $x_0, x_1, \cdots, x_n$ as the zeros of the Legendre polynomial (called Gauss points) $\phi_{n+1}(x)$ so that

$$\phi_{n+1}(x) = c_{n+1} \prod_{i=0}^{n} (x - x_i).$$

- If $f(x)$: is a polynomial of degree $2n+1$, then $f[x_0, x_1, \cdots, x_n, x]$: is a polynomial of degree n, and
- $E(f) = \int_a^b f[x_0, x_1, \cdots, x_n, x] \prod_{i=0}^{n} (x - x_i) dx = 0$
- Thus, we have achieved highest precision of $2n+1$
- The resulting methods are called **Gaussian quadrature**.

Gaussian Quadrature

Example: $a = -1$ and $b = 1$. Then

$$\phi_0(x) = 1,\ \phi_1(x) = x,\ \phi_2(x) = \frac{1}{2}(3x^2 - 1),\ \phi_3(x) = \frac{1}{2}(5x^3 - 3x), \cdots$$

- $n = 0$: $\phi_1(x) = x \implies x_0 = 0$. $w_0 = 2$, the mid-point rule:

$$\int_{-1}^{1} f(x)dx \approx 2f(0)$$

  precision=?

- $n = 1:\ x_0 = -\frac{1}{\sqrt{3}},\ x_1 = \frac{1}{\sqrt{3}}$, and $w_0 = w_1 = 1$

$$\int_{-1}^{1} f(x)dx \approx f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}})$$

  precision=?

Gaussian Quadrature

- $n = 2: \quad x_0 = -\sqrt{\frac{3}{5}}, x_1 = 0, x_2 = \sqrt{\frac{3}{5}},\ w_0 = w_2 = \frac{5}{9}$, and $a_1 = 2 - 2w_0 = \frac{8}{9}$

$$\int_{-1}^{1} f(x)dx \approx ?$$

precision=?

Gaussian Quadrature

On the canonical interval $[-1, 1]$ for a given $n \in \mathbb{N}$:

- The *Gauss points* are the zeros of the Legendre polynomial of degree $n+1$, $\phi_{n+1}(x)$.
- The corresponding quadrature weights are

$$w_j = \frac{2(1 - x_j^2)}{[(n+1)\phi_n(x_j)]^2}, \quad j = 0, 1, \cdots, n$$

- The corresponding error is

$$\int_{-1}^{1} f(x)dx - \sum_{j=0}^{n} w_j f(x_j) = \frac{2^{2n+3}((n+1)!)^4}{(2n+3)!((2n+2)!)^2} f^{(2n+2)}(\xi)$$

For the interval $[a, b]$, the affine transformation

$$t = \frac{b-a}{2}x + \frac{b+a}{2}, \quad -1 \leq x \leq 1$$

Gaussian Quadrature

$$\int_a^b f(t)dt = \int_{-1}^1 f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right)\frac{b-a}{2}dx$$

then we have

$$\int_a^b f(t)dt \approx \sum_{j=0}^n b_j f(t_j)$$

where

- $$t_j = \frac{b-a}{2}x_j + \frac{b+a}{2}$$

- $$b_j = \frac{b-a}{2}w_j$$

Gaussian Quadrature

Example: Integrate $\int_0^1 e^{-x^2} dx$ using Gaussian Quadrature with $n = 1$, and $n = 2$.

Composite Gaussian rule:

$$a = t_0 < t_1 < \cdots < t_r = b,$$

where $h = \frac{b-a}{r}$. The error in the composite Gaussian rule is estimated by

$$E_{n,h}(f) = \frac{(b-a)((n+1)!)^4}{(2n+3)!((2n+2)!)^2} f^{(2n+2)}(\xi) h^{2n+2}.$$

Two-point composite Gaussian method vs. composite Simpson method:

- Simpson method has simplicity of equal subintervals.
- Gauss method has a somewhat better error constant.
  - Requires one less function evaluation.
  - shows more flexibility with discontinuities in the integrand.

Gaussian Quadrature

Consider the integral $I_f = \int_0^{2\pi} f(x)dx$, where

$$f(x) = \begin{cases} \sin(x), & 0 \leq x \leq \frac{\pi}{2} \\ \cos(x), & \frac{\pi}{2} < x \leq 2\pi. \end{cases}$$

Basic rules provide $O(1)$ error.

- $I_{mid} = -2\pi$
- $I_{Simp} = \pi$

With a breakpoint at the discontinuity location $x = \frac{\pi}{2}$

Method	# subintervals	Fevals	Error
Midpoint	4	4	5.23×10^{-16}
Trapezoidal	4	5	7.85×10^{-1}
Trapezoidal	8	9	3.93×10^{-1}
Gauss, $n = 1$	4	8	4.56×10^{-16}
Simpson	4	9	2.62×10^{-1}
Simpson	8	17	1.31×10^{-1}