Numerical Integration

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- Not all functions have closed-form anti-derivatives. Thus not all integrals can be evaluated by the Fundamental Theorem of Calculus.
- For special functions, such as the error function

$$\frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt,$$

  efforts can be taken to tabulate values once for all. But this practice is too limited.

- One better approach is to approximate the integral by quadratures.
  - Given a function $f(t)$ defined on $[a, b]$, a formula of the form

$$Q_n(f) := \sum_{i=1}^{n} \alpha_i f(x_i) \tag{1}$$

  with $\alpha_i \in R$ and $x_i \in [a, b]$ is called a quadrature rule for the integral $I(f) := \int_a^b f(t)dt$.
    - The points x_i are called the quadrature points (abscissas)
    - The values α_i are called the quadrature coefficients (weights).
    - The quadrature error is defined to be $E_n(f) := I(f) - Q_n(f)$.

- A quadrature rule is said to have degree of precision m if $E_n(x^k) = 0$ for $k = 0, \ldots, m$ and $E_n(x^{m+1}) \neq 0$.
  - If a quadrature rule has degree of precision m, then $E_n(p_k) = 0$ for all polynomials $p_k(x)$ of degree $\leq m$.
- The trapezoidal rule,

$$Q_2(f) = \frac{b-a}{2}[f(a) + f(b)], \tag{2}$$

is a quadrature rule with degree of precision $m = 1$.
(Try to prove this by graph.)

- Recall the linear interpolant of $f(t)$ and the corresponding error:

$$f(t) = f(a) + \frac{f(b) - f(a)}{b - a}(t - a) + \frac{f''(\xi_t)}{2}(t - a)(t - b).$$

- Integrate both side of the above, we obtain

$$I(f) \approx Q_2(f) = \frac{b - a}{2}[f(a) + f(b)]$$

and

$$E_2(f) = \int_a^b \frac{f''(\xi_t)}{2}(t - a)(t - b)dt.$$

- Recall the Mean Value Theorem for integrals: *If f is continuous and g is nondecreasing in the interval $[a, b]$, then there exists $\xi \in [a, b]$ such that*

$$\int_a^b f dg = f(\xi) \int_a^b dg.$$

- We may rewrite

$$E_2(f) = \frac{f''(\eta)}{2} \int_a^b (t-a)(t-b)dt = -\frac{f''(\eta)}{12}(b-a)^3. \tag{3}$$

- If $|f''(t)|$ is not too large and if $b-a$ is small, the trapezoidal rule gives an approximation with errors around $O(h^3)$.

- Over a large interval, the trapezoidal rule should be applied by summing the results of many applications of the rule over smaller intervals. This is called **composite trapezoidal rule**.
  - Divide $[a, b]$ into n equally spaced intervals with step size $h = \frac{b-a}{n}$ and nodes $x_i = a + ih$ for $i = 0, 1, \ldots, n$.
  - Use the trapezoidal rule to approximate

$$\int_{x_{i-1}}^{x_i} f(x)dx \approx \frac{h}{2}[f(x_{i-1}) + f(x_i)]$$

    over each subinterval $[x_{i=1}, x_i]$.
  - Sum these approximations together:

$$\int_a^b f(x)dx \approx h\left[\frac{f(x_0)}{2} + f(x_1) + \ldots + f(x_{n-1}) + \frac{f(x_n)}{2}\right]. \tag{4}$$

    This is called the composite trapezoidal rule.

Lemma (Discrete Mean-Value Theorem)

Let $u \in C^0([a,b])$ and let x_j be $k+1$ points in $[a,b]$ and a_j be $k+1$ constants, all having the same sign. Then there exists $\eta \in [a,b]$ such that

$$\sum_{j=0}^{k} a_j u(x_j) = u(\eta) \sum_{j=0}^{k} a_j.$$

Proof.

Without loss of generality, assume $a_j \geq 0$ for all j. Let $F(x) = \sum_{j=0}^{k} a_j u(x)$, $u(\bar{x}) = \min_{x \in [a,b]} u(x)$, and $u(\bar{\bar{x}}) = \max_{x \in [a,b]} u(x)$. It follows that

$$F(\bar{x}) \leq \sum_{j=0}^{k} a_j u(x_j) \leq F(\bar{\bar{x}}).$$

Since F is continuous on $[a,b]$, there exists $\eta \in [a,b]$ such that

$$F(\eta) = \sum_{j=0}^{k} a_j u(x_j).$$

- Error formula for the composite trapezoidal rule :

$$E_n(f) = -\frac{h^3}{12}\sum_{i=1}^{n} f''(\eta_i) = -\frac{h^2}{12}\frac{b-a}{n}\sum_{i=1}^{n} f''(\eta_i) = -\frac{(b-a)h^2}{12}f''(\eta).$$

- The way the trapezoidal rule is derived can be generalized to higher degree polynomial interpolants. Such a quadrature rule is called a **Newton-Cotes formula**.
- Let $x_0, x_1, \ldots, x_n$ be given nodes in $[a, b]$. Recall that the Lagrange interpolation of a function at these nodes is given by the polynomial

$$p(t) = \sum_{j=0}^{n} f(x_j)\ell_j(t)$$

where each $\ell_j(t)$ is the Lagrange polynomial

$$\ell_j(t) := \prod_{i=0, i \neq j}^{n} \frac{t - x_i}{x_j - x_i}, \; j = 0, 1, \ldots, n.$$

- We therefore have

$$\int_a^b f(t)dt \approx \int_a^b p(t)dt = \sum_{j=0}^{n} \omega_j f(x_j)$$

where the weight ω_j is determined by

$$\omega_j = \int_a^b \ell_j(t)dt. \tag{5}$$

  - Note that if $f(t)$ itself is a polynomial of degree $\leq n$, then

$$f(t) = \sum_{j=0}^{n} f(x_j)\ell_j(t). \text{ (Why?)}$$

    In this case, the Newtow-Cotes quadrature rule evaluates $\int_a^b f(t)dt$ precisely.
  - The Newton-Cotes quadrature rule has degree of precision at least n.

- It is nice to know how the weight ω_j should be calculated. However, there are some other concerns:
  - These weights are difficult to evaluate.
  - How high can the degree of precision be pushed?
- Suppose we approximate $f(t)$ by a quadratic polynomial $p_2(t)$ that interpolates $f(a), f\left(\frac{a+b}{2}\right)$ and $f(b)$.
  - It can be shown that

$$Q_3(f) = \frac{b-a}{6}[f(a) + 4f(\frac{a+b}{2}) + f(b)].\text{(Do it now.)}$$

  - Compute $\ell_0(x) = \frac{(x-\frac{a+b}{2})(x-b)}{(a-b)^2/2}, \ell_1(x) = \ldots, \ell_2(x) = \ldots$

- The error part is tricky!
  - Observe that the function (in variable s) from Newton's formula, $g(s) = p_2(s) + f[a, b, \frac{a+b}{2}, t](s-a)(s-b)(s-\frac{a+b}{2})$, interpolates f at $a, b, \frac{a+b}{2}$ and t.
    - $p_2(s)$: polynomial of degree 2.
  - Taking s as t and Thinking t as arbitrary, we should have

$$f(t) = p_2(t) + f[a, b, \frac{a+b}{2}, t](t-a)(t-b)(t-\frac{a+b}{2})$$

  - The error $E_3(f)$ therefore is given by

$$E_3(f) = \int_a^b f[a, b, \frac{a+b}{2}, t]\omega(t)dt \qquad (6)$$

    with $\omega(t) := (t-a)(t-b)(t-\frac{a+b}{2})$.
  - We already know that the degree of precision is ≥ 2. Can this be better?

- Here, we analyze $E_3(f)$ by the method of integration by parts.
  - Let $\Omega(x) := \int_a^x \omega(t)dt$. Then $\Omega'(x) = \omega(x)$.
  - By integration by parts, we have

$$E_3(f) = f[a, b, \frac{a+b}{2}, x]\Omega(x)|_a^b - \int_a^b f[a, b, \frac{a+b}{2}, x, x]\Omega(x)dx.$$

    - $f[a, a+h] = \frac{f(a+h)-f(a)}{h}$.
    - $f[a, a] = \lim_{h\to 0} \frac{f(a+h)-f(a)}{h} = f'(a)$.

- Observe that $\Omega(a) = \Omega(b) = 0$. Observe also that $\Omega(x) > 0$ for all $x \in (a, b)$.
- We may apply the mean value theorem to conclude that

$$\begin{aligned} E_3(f) &= -\int_a^b f[a, b, \frac{a+b}{2}, x, x]\Omega(x)dx \\ &= -f[a, b, \frac{a+b}{2}, \xi, \xi] \int_a^b \Omega(x)dx \\ &= -\frac{f^{(4)}(\eta)}{4!}\frac{4}{15}\left(\frac{b-a}{2}\right)^5 \\ &= -\frac{f^{(4)}(\eta)}{90}\left(\frac{b-a}{2}\right)^5. \end{aligned}$$

- The degree of precision for Simpson's rule is 3 rather than 2.

- Divide the interval into $2n$ equally space subintervals with $h = \frac{b-a}{2n}$ and $x_i = a + ih$ for $i = 0, 1, \ldots, 2n$. Upon applying Simpson's rule over two consecutive subintervals $[x_{2j}, x_{2j+2}]$ for $j = 0, 1, \ldots, n-1$ and summing up these integrals, we obtain the composite Simpson's rule:

$$\int_a^b f(t)dt \approx \frac{h}{3}\left\{f_0 + 4f_1 + 2f_2 + 4f_3 + \ldots + 2f_{2n-2} + 4f_{2n-1} + f_{2n}\right\}. \qquad (7)$$

  - The error formula for the composite Simpson's rule can be obtained in the same way as we derived the error formula for the composite trapezoidal rule:

$$\begin{aligned} E_{3,cs} &= \sum_{i=1}^{n} -\frac{f^{(4)}(\eta_i)}{90} h^5 = -\frac{(b-a)h^4}{180n} \sum_{i=1}^{n} f^{(4)}(\eta_i) \\ &= -\frac{(b-a)h^4}{180} f^{(4)}(\eta). \end{aligned}$$

- An improper integral such as $\int_0^1 \frac{1}{\sqrt{t}} dt$ does exist even though it is not defined at $t = 0$.
  - A Newton-Cotes quadrature must exclude the node $t = 0$. Even so, the results are not good. (Why?)
  - A better approach is to incorporate the singularity into the quadrature rule itself.
- The idea is to integrate a function $f(t)$ with respect to a specified weight function $w(x)$, i.e.,

$$I_w(f) := \int_a^b f(t)w(t)dt \tag{8}$$

where $w(t) \geq 0$ on $[a, b]$. In such a case, we consider a quadrature rule of the form

$$Q_w(f) := \sum_{i=1}^{n} \alpha_i f(x_i). \tag{9}$$

  - Note that the weight function $w(x)$ does not appear on the right hand side of (9).

- An example: Suppose $w(t) = t^{-1/2}$ and suppose the nodes selected are $x_1 = \frac{1}{4}$ and $x_2 = \frac{3}{4}$. We want to determined the coefficients α_1 and α_2 in the quadrature so that

$$\begin{aligned}
\int_0^1 1 t^{-1/2} dt = 2 &= \alpha_1 + \alpha_2 \\
\int_0^1 t t^{-1/2} dt = \frac{2}{3} &= \frac{1}{4}\alpha_1 + \frac{3}{4}\alpha_2 .
\end{aligned}$$

  - The newly weighted quadrature reads like

$$\int_0^1 f(t) t^{-1/2} dt \approx \frac{5}{3} f(\frac{1}{4}) + \frac{1}{3} f(\frac{3}{4}).$$

  - The entire theory that works for Newton-Cotes or Gaussian quadratures can be generalized to the weighted integrals. The arguments will not be repeated in this course, but take note of this possibility.

- Newton-Cotes quadratures for the integral $I(f) = \int_a^b f(x)dx$ are based on the integration of the polynomial $p(x)$ that interpolates $f(x)$ at a set of pre-selected nodes in $[a, b]$.
  - The weights of a Newton-Cotes are determined by $\omega_j = \int_a^b \ell_j(t)dt$.
  - It can be proved that (Theorem 9.2) the degree of precision for a Newton-Cotes formula of equally spaced nodes $x_0, x_1, \ldots, x_n$ is
    1. $n + 1$, if n is even (such as Simplson's rule).
    2. n, if n is odd (such as the trapezoidal rule).

- Gaussian quadratures adopt a different approach in which both the abscissas x_i and weights α_i are to be determined simultaneously so that the quadrature

$$Q_n(f) = \sum_{i=1}^{n} \alpha_i f(x_i) \tag{10}$$

  has a maximal degree of precision.
  - Since there are $2n$ unknowns in (10), the requirements

$$E_n(x^k) = 0, k = 0, 1, \ldots, 2n-1 \tag{11}$$

    supply $2n$ equations.
  - It is expected that the maximal degree of precision is $\geq 2n - 1$.
- To determine the Gaussian quadrature, one approach is through the orthogonal polynomials.

- Two functions f and g defined on $[a, b]$ are said to be orthogonal if and only if

$$\langle f, g \rangle := \int_a^b f(t)g(t)dt = 0. \tag{12}$$

  - The operation $\langle f, g \rangle$ may be regarded as an inner product of f and g.
  - A sequence $\{p_i(t)\}_{i=0}^{\infty}$ of polynomials with $\deg(p_i) = i$ is called a sequence of orthogonal polynomials on $[a, b]$ if

$$\int_a^b p_i(t)p_j(t)dt = 0, \quad \text{whenever } i \neq j.$$

    - The orthogonality is not affected by scalar multiplication. We may assume that all $p_i(t)$ are monic, i.e., the leading coefficients of all $p_i(t)$ are one.
    - Any n-th degree polynomial $q(t)$ can uniquely be written as

$$q(t) = b_n p_n(t) + b_{n-1} p_{n-1}(t) + \ldots + b_0 p_0(t).$$

      That is, the orthogonal polynomials of degree $\leq n$ span the entire space of polynomials of degree $\leq n$.

- The following process constructs orthogonal polynomials over an arbitrary $[a, b]$:
  - $p_0(t) = 1$.
  - $p_1(t) = t - a_1$, but
  $$0 = \langle p_0, p_1 \rangle \implies a_1 = \frac{b+a}{2}.$$
  - Suppose $p_0(t), \ldots p_n(t)$ has been constructed. We seek $p_{n+1}(t)$ in the form
  $$p_{n+1}(t) = (t - a_{n+1})p_n(t) + b_{n+1}p_{n-1}(t) + c_{n+1}p_{n-2}(t) + \ldots.$$

- a_{n+1} can be determined from

$$0 = \langle p_{n+1}, p_n \rangle \Longrightarrow a_{n+1} = \frac{\langle t, p_n^2 \rangle}{\langle p_n, p_n \rangle}.$$

- b_{n+1} can be determined from

$$0 = \langle p_{n+1}, p_{n-1} \rangle \Longrightarrow b_{n+1} = -\frac{\langle t, p_n p_{n-1} \rangle}{\langle p_{n-1}, p_{n-1} \rangle}.$$

- c_{n+1} can be determined from

$$0 = \langle p_{n+1}, p_{n-2} \rangle \Longrightarrow c_{n+1} = -\frac{\langle t, p_n p_{n-2} \rangle}{\langle p_{n-2}, p_{n-2} \rangle}.$$

But, surprisingly, the numerator $\langle t, p_n p_{n-2} \rangle = \langle p_{n-1}, p_n \rangle = 0$. (Why?)

- We therefore conclude that $p_{n+1}(t)$ can be generated by a three-term recurrence formula:

$$p_{n+1}(t) = (t - a_{n+1})p_n(t) + b_{n+1}p_{n-1}(t). \tag{13}$$

- If $[a, b] = [-1, 1]$, such a sequence of orthogonal polynomials are called the Legendre polynomials.

We are interested in deriving quadratures with higher degrees of precision. Toward this end, observe the following two facts:

Theorem

A quadrature formula using $n+1$ distinct abscissas has degree of precision $\geq n$ if and only if it results from the integration of an interpolation polynomial.

Proof.

$(\Longleftarrow)$

- This follows from Theorem 8.3.1 of Chu's note for MA780.

$(\Longrightarrow)$

- Suppose the quadrature rule is $Q_n(f) = \sum_{i=0}^{n} \alpha_i f(x_i)$.
- Following from the assumption, we have $\sum_{i=0}^{n} \alpha_i x_i^k = \frac{b^{k+1} - a^{k+1}}{k+1}$ for $k = 0, \ldots, n$.

- We may rewrite this system of equations as

$$\begin{bmatrix} 1 & \dots & 1 \\ x_0 & \dots & x_n \\ \vdots & & \\ x_0^n & \dots & x_n^n \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} b-a \\ \frac{b^2-a^2}{2} \\ \vdots \\ \frac{b^{n+1}-a^{n+1}}{n+1} \end{bmatrix}. \tag{14}$$

  The coefficient matrix is the Vandermonde matrix. Thus the system (14) has a unique solution for α_i, $i = 0, \dots, n$.
- On the other hand, we can construct an interpolating polynomial of degree n using the same nodes $\{x_i\}_{i=0}^n$.
- This polynomial results in a quadrature formula $\sum_{i=0}^{n} \beta_i f(x_i)$ which has degree of precision at least n. (Why?)
- By setting $E_n(x^k) = 0$ for $k = 0, \dots, n$ in the new quadrature, we end up with the same linear system (14).
- By uniqueness, it must be that $\alpha_i = \beta_i$. $\square$

Since the Gaussian quadrature is expected to have degree of precision higher than n, we conclude that

- It may be thought of as the integration of a certain polynomial that interpolates $f(x)$ at a certain set of nodes $x_0, \dots, x_n$.
- It must remain true that

$$E_{n+1}(f) = \int_a^b f[x_0, \dots, x_n, t] \prod_{i=0}^{n} (t - x_i) dt. \tag{15}$$

- Not only $E_{n+1}(x^k) = 0$ for $k = 0, \dots, n$, but we further would like to require $E_{n+1}(x^k) = 0$ for $k = n+1, \dots, n+\nu$, and for ν as large as possible.

Theorem

If $f(t) = t^{(n+1)+\nu}, \nu \geq 0$, then the $(n+1)$-th divided difference $f[x_0, \ldots, x_n, t]$ is a polynomial of degree at most ν.

Proof.

- When $n = 0$, we find $f[x_0, t] = \frac{f(x_0)-f(t)}{x_0-t} = \frac{x_0^{1+\nu}-t^{1+\nu}}{x_0-t}$ is obviously a polynomial of degree ν.
- Suppose the assertion is true for $n = k$. Consider $f(t) = t^{[(k+1)+1]+\nu}$. (We are preparing to use the Induction Principle on n.)
- Regard $f(t) = t^{(k+1)+(1+\nu)}$. Then, by induction hypothesis, the difference quotient $f[x_1, \ldots, x_{k+1}, t]$ is a polynomial of degree at most $\nu + 1$.
- Observe that

$$f[x_0, \ldots, x_{k+1}, t] = \frac{f[x_0, \ldots, x_{k+1}] - f[x_1, \ldots, x_{k+1}, t]}{x_0 - t}.$$

  Note that the numerator has a zero at $t = x_0$. After cancelation, $f[x_0, \ldots, x_{k+1}, t]$ is a polynomial of degree of most ν.
- The assertion now follows from the induction. □

- Recall that
  - The Gaussian quadrature is a special type of Newton-Cotes quadrature.
  - The error in the quadrature is given by

$$E_{n+1}(f) = \int_a^b f[x_0, \ldots, x_n, t] \prod_{i=0}^{n} (t - x_i) dt.$$

  - The divided difference $f[x_0, \ldots, x_n, t]$ is a polynomial of degree at most ν if $f(t) = t^{(n+1)+\nu}$.
  - If we can choose the nodes x_i so that $\omega(t) = \prod_{i=0}^{n} (t - x_i)$ is the $(n+1)$-th orthogonal polynomials, then the error $E(t^{(n+1)+\nu}) = 0$ for all $\nu = 0, 1, \ldots, n$.

- Need to make sure all roots of the n-th orthogonal polynomial are real-valued, distinct, and contained in (a, b).
  - Let $x_0 \ldots, x_m \in (a, b)$ denote all the distinct, real zeros of $\omega_n(x)$ with odd multiplicity.
  - Assume $m < n$. We want to prove by contradiction.
  - Consider the integral $\int_a^b (x - x_0) \ldots (x - x_m)\omega_n(x)dx$. Note that the integrand does not change sign over $[a, b]$ and is not identically zero. Thus the integral is positive.
  - But $(x - x_0) \ldots (x - x_m)$ is a polynomial of degree $m < n$.
  - By orthogonality of $\omega_n(x)$, the integral should be zero. This is a contradiction.
  - It must be that $m = n$, and the multiplicity is 1.

- Gaussian abscissas and weights over the interval $[-1, 1]$.

n	Abscissas x_j	Weights α_j
1	$\pm 1/\sqrt{3}$	1
2	$\pm\sqrt{0.6}$	5/9
	0	8/9
3	± 0.8611363116	0.3478548451
	± 0.3399810436	0.6521451549
4	± 0.9061798459	0.2369268850
	± 0.5384693101	0.4786286705
	0	0.5688888889
5	± 0.9324695142	0.1713244924
	± 0.6612093865	0.3607615730
	± 0.2386191861	0.4679139346

- To integrate $f(x)$ over an arbitrary interval $[a, b]$,
  - Change of variables:

$$x = a + \frac{b-a}{2}(\xi + 1), \; dx = \frac{b-a}{2} d\xi.$$

  - Substitution:

$$\begin{aligned}
\int_a^b f(x)dx &= \int_{-1}^{1} f(a + \frac{b-a}{2}(\xi + 1))\frac{b-a}{2} d\xi \\
&= \frac{b-a}{2} \int_{-1}^{1} f(a + \frac{b-a}{2}(\xi + 1))d\xi \\
&\approx \frac{b-a}{2} \sum_{i=1}^{n} \alpha_i f(x_i)
\end{aligned}$$

    - α_j are the tabulated Gaussian weights associated with the tabulated Gaussian abscissa ξ_j in $[-1, 1]$.
    - x_j is obtained from ξ_j through $x_j = a + \frac{b-a}{2}(\xi_j + 1), \; j = 0, \ldots, n$.