MA 8020: Numerical Analysis II
Numerical Differentiation and Integration

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Introduction

If the values of a function f are given at a few points $x_0, x_1, \cdots, x_n$, can that information be used to estimate a derivative

$$f'(c)$$

or an integral

$$\int_a^b f(x)dx?$$

Numerical differentiation

- Assume that $h > 0$ and $f \in C^2[x, x+h]$. By Taylor's Theorem, we have
$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi),$$
for some $\xi \in (x, x+h)$. Rearranging the expansion, we obtain
$$f'(x) = \frac{1}{h}\Big(f(x+h) - f(x)\Big) - \frac{h}{2} f''(\xi).$$

- If the term $-\frac{h}{2} f''(\xi)$ is small, then we have an approximation of $f'(x)$,
$$f'(x) \approx \frac{1}{h}\Big(f(x+h) - f(x)\Big).$$
The term "$-\frac{h}{2} f''(\xi)$" is called the truncation error.

Example

Let $f(x) = \cos(x)$, $x = \pi/4$ and $h = 0.01$.

We know the exact solution is $f'(\frac{\pi}{4}) = -\sin(\frac{\pi}{4}) \cong -0.7071$.

$$\begin{aligned} \frac{1}{h}\Big(f(x+h) - f(x)\Big) &= \frac{1}{0.01}\Big(0.700000476 - 0.707106781\Big) \\ &= -0.71063051. \end{aligned}$$

- True error: $|-0.7071 - (-0.7106)| = 0.0035.$
- Truncation error: $|-\frac{h}{2}f''(\xi)| = 0.005|\cos(\xi)| \leq 0.005.$

Subtractive cancelation

- **Question:** *can we get a smaller error by using a smaller step size h?*
- **Example:** consider $f(x) = \tan^{-1}(x)$ at $x = \sqrt{2}$. We know that the exact solution is $f'(x) = (x^2+1)^{-1}$ and $f'(\sqrt{2}) = \frac{1}{3}$.

h	$f(x)$	$f(x+h)$	$f'(x) \approx$
0.62×10^{-1}	0.95531660	0.97555095	0.32374954
0.24×10^{-3}	0.95531660	0.95539796	0.33325195
0.95×10^{-6}	0.95531660	0.95531690	0.31250000
0.60×10^{-7}	0.95531660	0.95531666	1.00000000
0.15×10^{-7}	0.95531660	0.95531660	0.00000000

- When h is too small, $f(x)$ and $f(x+h)$ are too close to each other, the significant digits were canceled.
- One resolution is to use a higher order method. h doesn't need to be too small.

Higher order methods

- Assume that $h > 0$ and $f \in C^3[x-h, x+h]$. By Taylor's Theorem, we have

$$
\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(\xi_1), \\
f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(\xi_2),
\end{aligned}
$$

  for some $\xi_1 \in (x, x+h)$ and $\xi_2 \in (x-h, x)$. After subtracting and rearranging, we have

$$
f'(x) = \frac{1}{2h}\Big(f(x+h) - f(x-h)\Big) - \frac{h^2}{6}\frac{1}{2}\Big(f'''(\xi_1) + f'''(\xi_2)\Big).
$$

- This is a more favorable result, because of the h^2 term in the error. Notice, however, the presence of f''' in the error.

Higher order methods (cont'd)

- From the Intermediate Value Theorem, we have that there is a $\xi \in (x-h, x+h)$, such that

$$f'''(\xi) = \frac{1}{2}\Big(f'''(\xi_1) + f'''(\xi_2)\Big).$$

Hence,

$$f'(x) = \frac{1}{2h}\Big(f(x+h) - f(x-h)\Big) - \frac{h^2}{6}f'''(\xi).$$

Therefore,

$$f'(x) \approx \frac{1}{2h}\Big(f(x+h) - f(x-h)\Big),$$

which is a second order formula.

Example

Consider $f(x) = \tan^{-1}(x)$ at $x = \sqrt{2}$. We know that the exact solution is $f'(x) = (x^2+1)^{-1}$ and $f'(\sqrt{2}) = \frac{1}{3}$.

h	$f(x-h)$	$f(x+h)$	$f'(x) \approx$
0.25×10^{0}	0.86112982	1.02972674	0.33719385
0.9765×10^{-3}	0.95499092	0.95564199	0.33334351
0.3815×10^{-5}	0.95531535	0.95531786	0.32812500
0.1490×10^{-7}	0.95531660	0.95531660	0.00000000

Approximation of $f''(x)$

Assume that $h > 0$ and $f \in C^4[x-h, x+h]$. From Taylor's Theorem, we have

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(\xi_1), \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(\xi_2), \end{aligned}$$

for $\xi_1 \in (x, x+h)$ and $\xi_2 \in (x-h, x)$. After sum and rearrangement, we obtain the following central difference formula:

$$\begin{aligned} f''(x) &= \frac{1}{h^2}\Big(f(x+h) - 2f(x) + f(x-h)\Big) - \frac{h^2}{12}\frac{1}{2}\Big(f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\Big) \\ &= \frac{1}{h^2}\Big(f(x+h) - 2f(x) + f(x-h)\Big) - \frac{h^2}{12}f^{(4)}(\xi), \end{aligned}$$

where at the last equality we use the Intermediate Value Theorem again. Thus, we have a second order approximation of $f''(x)$

$$f''(x) \approx \frac{1}{h^2}\Big(f(x+h) - 2f(x) + f(x-h)\Big).$$

Homework

Derive the following two formulas for approximating derivatives and show that they are both $O(h^4)$ by establishing their error terms:

$$
\begin{aligned}
f'(x) &\approx \frac{1}{12h}\Big(-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)\Big), \\
f''(x) &\approx \frac{1}{12h^2}\Big(-f(x+2h)+16f(x+h)-30f(x) \\
&\qquad +16f(x-h)-f(x-2h)\Big).
\end{aligned}
$$

(see Textbook, page 477, #6)

Differentiation via polynomial interpolation

Goal: *given f at $n+1$ points $x_0, x_1, \cdots, x_n$. We wish to compute $f'(x_\alpha)$, where x_α is any of the node points.*

- We interpolate f with a polynomial, its Lagrange form is

$$f(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=0}^{n}(x - x_i).$$

Define $w(x) = \prod_{i=0}^{n}(x - x_i)$.

- Taking the above equation derivative, we obtain

$$\begin{aligned} f'(x) &= \sum_{i=0}^{n} f(x_i)\ell_i'(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w'(x) \\ &\quad + \frac{1}{(n+1)!} w(x) \frac{d}{dx} f^{(n+1)}(\xi_x). \end{aligned}$$

Hence,

$$f'(x_\alpha) = \sum_{i=0}^{n} f(x_i)\ell_i'(x_\alpha) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{j=0, j\neq\alpha}^{n}(x_\alpha - x_j).$$

Example

- Use the equation above when $n = 1$ and $\alpha = 0$. The two Lagrange cardinal functions are

$$\ell_0(x) = \frac{x - x_1}{x_0 - x_1} \quad \text{and} \quad \ell_1(x) = \frac{x - x_0}{x_1 - x_0}.$$

Their derivatives are

$$\ell_0'(x) = \frac{1}{x_0 - x_1} = \frac{-1}{h} \quad \text{and} \quad \ell_1'(x) = \frac{1}{x_1 - x_0} = \frac{1}{h}.$$

- Hence we have

$$f'(x_0) = \frac{-f(x_0)}{h} + \frac{f(x_1)}{h} + \frac{1}{2}f''(\xi_x)(x_0 - x_1),$$
$$\Longrightarrow f'(x_0) = \frac{f(x_1) - f(x_0)}{h} - \frac{h}{2}f''(\xi_x).$$

Richardson extrapolation

- Richardson extrapolation is a general procedure to improve accuracy.
- Assume that f is sufficiently smooth and

$$f(x+h)=\sum_{k=0}^{\infty}\frac{1}{k!}h^k f^{(k)}(x) \quad \text{and} \quad f(x-h)=\sum_{k=0}^{\infty}\frac{1}{k!}(-1)^k h^k f^{(k)}(x).$$

After subtraction and rearrangement, we obtain

$$\begin{aligned} f'(x) &= \frac{1}{2h}\big(f(x+h)-f(x-h)\big) \\ &\quad -\left(\frac{1}{3!}h^2 f^{(3)}(x)+\frac{1}{5!}h^4 f^{(5)}(x)+\frac{1}{7!}h^6 f^{(7)}(x)+\cdots\right), \end{aligned}$$

or in an abstract form

$$L=\phi(h)+\left(a_2h^2+a_4h^4+a_6h^6+\cdots\right).$$

Richardson extrapolation (cont'd)

- We rewrite the formula in the previous page as

$$L = \phi(h) + \left(a_2 h^2 + a_4 h^4 + a_6 h^6 + \cdots\right). \qquad (*)$$

If $a_2 \neq 0$, the truncation error is $O(h^2)$. How can we get rid of this term? Rewrite the abstract form for $h/2$ to get

$$L = \phi(\frac{h}{2}) + \left(\frac{a_2}{4}h^2 + \frac{a_4}{16}h^4 + \frac{a_6}{64}h^6 + \cdots\right). \qquad (**)$$

Multiplying $(**)$ by 4 and subtracting from $(*)$, we obtain

$$L = \frac{4}{3}\phi(\frac{h}{2}) - \frac{1}{3}\phi(h) - \left(\frac{a_4}{4}h^4 + \frac{5a_6}{16}h^6 + \cdots\right).$$

- This formula is the first step in Richardson extrapolation. It shows that a simple combination of $\phi(h)$ and $\phi(h/2)$ furnishes an estimate of L with accuracy $O(h^4)$.

Numerical integration

Question: *How to compute $\int_a^b f(x)dx$ numerically?*

- If we know the antiderivative of f, say $F(x)$, then we have

$$\int_a^b f(x)dx = F(b) - F(a).$$

- Otherwise, we can find an approximation of $f(x)$, say $g(x)$ whose integral is easy to compute. Then

$$\int_a^b f(x)dx \approx \int_a^b g(x)dx.$$

Integration using polynomial interpolation

- We select some interpolation points $x_0, x_1, \cdots, x_n$ in $[a, b]$, and define the Lagrange interpolation of f,

$$g(x) = p(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x),$$

where ℓ_i, $i = 1, 2, \cdots, n$, are the cardinal functions,

$$\ell_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}, \quad \text{for } i = 0, 1, \cdots, n.$$

- Then we have

$$\int_a^b f(x)dx \approx \int_a^b p(x)dx = \int_a^b \sum_{i=0}^{n} f(x_i)\ell_i(x)dx = \sum_{i=0}^{n} f(x_i) \int_a^b \ell_i(x)dx.$$

Integration using polynomial interpolation (cont'd)

- Let us denote

$$A_i = \int_a^b \ell_i(x)dx,$$

which is independent of $f(x)$. Then we have a numerical integration formula:

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i).$$

- If the interpolation points are *equally spaced*, then this is called a Newton-Cotes formula.

Trapezoid rule

- If $n = 1$ and the interpolation points are $x_0 = a$, and $x_1 = b$. Then we have

$$\ell_0(x) = \frac{x-b}{a-b} \quad \textit{and} \quad \ell_1(x) = \frac{x-a}{b-a}.$$

$$A_0 = \int_a^b \frac{x-b}{a-b} = \frac{1}{2}(b-a) \quad \text{and} \quad A_1 = \int_a^b \frac{x-a}{b-a} = \frac{1}{2}(b-a).$$

- The corresponding quadrature formula is

$$\int_a^b f(x)dx \approx \frac{1}{2}(b-a)\Big(f(a)+f(b)\Big) \Longrightarrow \text{trapezoid rule.}$$

Error term in the trapezoid rule

- **The error term in the trapezoid rule:** Assume that $f \in C^2[a,b]$. Using the error term in the Lagrange interpolation and the mean-value theorem for integrals, we have

$$\int_a^b f(x) - p(x)dx = \int_a^b f''(\xi_x)\frac{(x-a)(x-b)}{2}dx$$

$$= -\frac{1}{2}f''(\xi)\int_a^b -x^2 + (a+b)x - abdx = \cdots = -\frac{1}{12}(b-a)^3 f''(\xi),$$

  where $f''(\xi_x) = 2(f(x) - p(x))/(x^2 - (a+b)x + ab)$ is continuous on (a,b) and can be continuously extended to $[a,b]$ by using the L'Hospital rule to calculate $\lim_{x\to a^+} f''(\xi_x)$ and $\lim_{x\to b^-} f''(\xi_x)$.

- The trapezoid rule is exact for all $f \in \Pi_1$. The error is large if the interval size is large.

- **The mean-value theorem for integrals** (cf. Textbook, page 19): *Assume that $u \in C[a,b]$, $v \in \mathcal{R}[a,b]$ and v doesn't change sign on $[a,b]$. Then $\exists\ \xi \in (a,b)$ such that $\int_a^b uv dx = u(\xi)\int_a^b v dx$.*

Composite trapezoid rule

- Partition the interval $[a, b]$ into $a = x_0 < x_1 < \cdots < x_n = b$, and then use the two-point trapezoid rule on each subinterval.

$$\int_a^b f(x)dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)dx \approx \frac{1}{2} \sum_{i=1}^{n} (x_i - x_{i-1}) \Big(f(x_{i-1}) + f(x_i) \Big).$$

- If the points are equally spaced, then we can introduce a step size $h = (b - a)/n$, where n is the number of subintervals. The interpolation points are $x_i = a + ih$. The composite trapezoid rule becomes

$$\int_a^b f(x)dx \approx \frac{h}{2} \Big(f(a) + 2 \sum_{i=1}^{n-1} f(x_i) + f(b) \Big).$$

Error term in the composite trapezoid rule

Assume that $f \in C^2[a,b]$. For uniform partition, the error term for the composite trapezoid rule is

$$\int_a^b f(x)dx - \frac{h}{2}\left(f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right) = -\frac{1}{12}(b-a)h^2 f''(\xi),$$

for some $\xi \in (a,b)$. ($\Longrightarrow$ exact for all $f \in \Pi_1$)

Proof. Using the error formula for the trapezoid rule, we have

$$\int_a^b f(x)dx - \frac{h}{2}\left(f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right) = \sum_{i=1}^{n} -\frac{1}{12}h^3 f''(\xi_i)$$

$$= -\frac{1}{12}h^2 \sum_{i=1}^{n} h f''(\xi_i) = -\frac{1}{12}h^2 \sum_{i=1}^{n} \frac{(b-a)}{n} f''(\xi_i)$$

$$= -\frac{1}{12}(b-a)h^2 \frac{1}{n}\sum_{i=1}^{n} f''(\xi_i) = -\frac{1}{12}(b-a)h^2 f''(\xi), \text{ for some } \xi \in (a,b),$$

where we use the intermediate value theorem for continuous functions at the last equality. □

Examples

- For example, if $n = 2$, and $[a, b] = [0, 1]$, then $x_0 = 0, x_1 = 0.5$, and $x_2 = 1$, we have $h = 1/2$. The composite trapezoid rule is

$$\int_0^1 f(x)dx \approx \frac{1}{4}f(0) + \frac{1}{2}f(0.5) + \frac{1}{4}f(1).$$

- If we take $n = 2$ and $[a, b] = [0, 1]$ in the Newton-Cotes procedure, we have

$$\int_0^1 f(x)dx \approx \frac{1}{6}f(0) + \frac{2}{3}f(0.5) + \frac{1}{6}f(1).$$

Solution:

$$\ell_0(x) = 2(x-0.5)(x-1),\ \ell_1(x) = -4x(x-1),\ \ell_2(x) = 2x(x-0.5),$$

$$A_0 = \int_0^1 \ell_0(x)dx = \frac{1}{6},\ A_1 = \int_0^1 \ell_1(x)dx = \frac{2}{3},\ A_2 = \int_0^1 \ell_2(x)dx = \frac{1}{6}.$$

(This formula is called Simpson's rule. It will be derived again by the method of undetermined coefficients below)

Recall the Newton-Cotes rule

- Recall the Newton-Cotes rule: $x_0 = a < x_1 < \cdots < x_n = b$, $h = x_i - x_{i-1}$ for all $i = 1, 2, \cdots, n$. *(equally spaced!)*

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i),$$

where

$$A_i = \int_a^b \ell_i(x)dx.$$

- This formula is exact for all $f \in \Pi_n$.

Method of undetermined coefficients

- Let us look at an example. For $n = 2$,

$$\int_0^1 f(x)dx \approx A_0 f(0) + A_1 f(0.5) + A_2 f(1).$$

- What are the coefficients A_0, A_1 and A_2? We seek the formula that will be exact for all polynomials of degree ≤ 2. It must be exact for $f(x) = 1, f(x) = x$ and $f(x) = x^2$, i.e.,

$$\begin{aligned} 1 &= \int_0^1 1dx = A_0 + A_1 + A_2, \\ \frac{1}{2} &= \int_0^1 xdx = \frac{1}{2}A_1 + A_2, \\ \frac{1}{3} &= \int_0^1 x^2dx = \frac{1}{4}A_1 + A_2. \end{aligned}$$

- Solving the 3×3 linear system, we obtain $A_0 = 1/6, A_1 = 2/3$, and $A_2 = 1/6$. This formula is called Simpson's rule on $[0, 1]$.

Simpson's rule

- If we repeat the previous exercise for the interval $[a, b]$, we have Simpson's rule on $[a, b]$:

$$\int_a^b f(x)dx \approx \frac{b-a}{6}\Big(f(a) + 4f(\frac{a+b}{2}) + f(b)\Big).$$

- We know that Simpson's rule is exact for all polynomials of degree ≤ 2. Surprisingly, Simpson's rule is exact for cubic polynomials.
- Let $[a, b] \subset (c, d)$. Assume that $f \in C^4[c, d]$. Then the error term of Simpson's rule is

$$-\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\xi), \quad \text{for some } \xi \in (a, b).$$

(See next three pages for the derivation)

- It is large if the interval size is large, but can be more accurate than the trapezoid rule if $b - a$ is small.

Error term of Simpson's rule

Let $h = (b-a)/2$. The numerical integration formula takes the form

$$\int_a^{a+2h} f(x)dx \approx \frac{h}{3}\Big(f(a) + 4f(a+h) + f(a+2h)\Big). \qquad (*)$$

Using Taylor's theorem, we have

$$\begin{aligned} f(a+h) &= f(a) + hf'(a) + \frac{h^2}{2!}f''(a) + \frac{h^3}{3!}f'''(a) + \frac{h^4}{4!}f^{(4)}(\xi_1), \\ f(a+2h) &= f(a) + 2hf'(a) + \frac{(2h)^2}{2!}f''(a) + \frac{(2h)^3}{3!}f'''(a) + \frac{(2h)^4}{4!}f^{(4)}(\xi_2), \end{aligned}$$

for some $\xi_1 \in (a, a+h)$ and $\xi_2 \in (a, a+2h)$. Substituting above equations into the right-hand side of (*) yields

$$\begin{aligned} &\frac{h}{3}\Big(f(a) + 4f(a+h) + f(a+2h)\Big) \qquad (**) \\ &= 2hf(a) + 2h^2f'(a) + \frac{4}{3}h^3f''(a) + \frac{2}{3}h^4f'''(a) \\ &\quad + \frac{1}{3}h\left(\frac{1}{3!}h^4f^{(4)}(\xi_1) + \frac{16}{4!}h^4f^{(4)}(\xi_2)\right). \end{aligned}$$

Error term of Simpson's rule (cont'd)

Define $F(x) := \int_a^x f(t)dt$ for $x \in [c,d]$. Then by the Fundamental Theorem of Calculus, part I, we have $F'(x) = f(x)$ for $x \in [a, a+2h]$. Using Taylor's theorem on the left-hand side of (*), we obtain

$$\int_a^{a+2h} f(x)dx = F(a+2h) = F(a) + (2h)F'(a) + \frac{(2h)^2}{2!}F''(a) \quad (***)$$
$$+\frac{(2h)^3}{3!}F'''(a) + \frac{(2h)^4}{4!}F^{(4)}(a) + \frac{(2h)^5}{5!}F^{(5)}(\eta)$$
$$= 0 + 2hf(a) + 2h^2 f'(a) + \frac{4}{3}h^3 f''(a) + \frac{2}{3}h^4 f'''(a) + \frac{32}{5!}h^5 f^{(4)}(\eta),$$

for some $\eta \in (a, a+2h)$. Comparing (**) and (***), we have

$$\begin{aligned}\int_a^{a+2h} f(x)dx &= \frac{h}{3}\Big(f(a) + 4f(a+h) + f(a+2h)\Big) \\ &\quad -\frac{1}{3}h\Big(\frac{1}{3!}h^4 f^{(4)}(\xi_1) + \frac{16}{4!}h^4 f^{(4)}(\xi_2)\Big) + \frac{32}{5!}h^5 f^{(4)}(\eta).\end{aligned}$$

Error term of Simpson's rule (cont'd)

Notice that Simpson's rule is exact for $f(x) = x^i$, $i = 0, 1, 2, 3$. Assume that

$$\int_a^{a+2h} f(x)dx = \frac{h}{3}\Big(f(a) + 4f(a+h) + f(a+2h)\Big) + Kf^{(4)}(\xi).$$

Using $f(x) = x^4$, we have $f^{(4)}(\xi) = 24$ and

$$\frac{1}{5}((a+2h)^5 - a^5) = \frac{h}{3}\Big(a^4 + 4(a+h)^4 + (a+2h)^4\Big) + 24K,$$

which implies

$$K = -\frac{h^5}{90}. \quad \square$$

Notice that

$$\begin{aligned}
&-\frac{1}{3}h\left(\frac{1}{3!}h^4 f^{(4)}(\xi_1) + \frac{16}{4!}h^4 f^{(4)}(\xi_2)\right) + \frac{32}{5!}h^5 f^{(4)}(\eta) \\
&= -\frac{1}{18}h^5 f^{(4)}(\xi_1) - \frac{2}{9}h^5 f^{(4)}(\xi_2) + \frac{4}{15}h^5 f^{(4)}(\eta) \\
&= \frac{-1}{90}h^5\Big(5f^{(4)}(\xi_1) + 20f^{(4)}(\xi_2) - 24f^{(4)}(\eta)\Big).
\end{aligned}$$

Composite Simpson's rule

- We partition the interval $[a, b]$ into n subintervals (even number) with $x_i = a + ih$, and $h = (b-a)/n$. Then,

$$\begin{aligned} \int_a^b f(x)dx &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx \\ &= \sum_{i=1}^{n/2} \int_{x_{2i-2}}^{x_{2i}} f(x)dx. \end{aligned}$$

  Using Simpson's rule on each interval $[x_{2i-2}, x_{2i}]$, we have

$$\begin{aligned} \int_a^b f(x)dx &\approx \frac{h}{3} \sum_{i=1}^{n/2} \Big(f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i}) \Big) \\ &= \frac{h}{3} \Big(f(x_0) + 2 \sum_{i=2}^{n/2} f(x_{2i-2}) + 4 \sum_{i=1}^{n/2} f(x_{2i-1}) + f(x_n) \Big). \end{aligned}$$

- The error is $-\frac{1}{180}(b-a)h^4 f^{(4)}(\xi)$ for some $\xi \in (a, b)$.

More general integration formulas

- Consider the definite integral

$$\int_a^b f(x)w(x)dx,$$

where $w(x)$ is a given weight function. For example $w(x) = \cos(x)$.

- We want a formula of the form

$$\int_a^b f(x)w(x)dx \approx \int_a^b \sum_{i=0}^{n} f(x_i)\ell_i(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i),$$

where

$$A_i = \int_a^b \ell_i(x)w(x)dx, \quad i = 0, 1, \cdots, n.$$

In general, A_i is hard to compute without using the method of undetermined coefficients.

More general integration formulas (cont'd)

- An important question to ask before using the method of undetermined coefficients: *what is highest degree of polynomials that the integration scheme can evaluate without error?*
- **Example:** Find a formula

$$
\begin{aligned}
\int_{-\pi}^{\pi} f(x)\cos(x)dx \;\approx\; & A_0 f\left(-\frac{3}{4}\pi\right) + A_1 f\left(-\frac{1}{4}\pi\right) \\
& + A_2 f\left(\frac{1}{4}\pi\right) + A_3 f\left(\frac{3}{4}\pi\right)
\end{aligned}
$$

  that is exact when f is a polynomial of degree 3. Since a polynomial of degree 3 is a linear combination of 4 polynomials $1, x, x^2$ and x^3, thus we can determine the four coefficients A_0, A_1, A_2, A_3 using the four conditions.

More general integration formulas (cont'd)

- An observation: the problem is symmetric! Therefore $A_0 = A_3$ and $A_1 = A_2$. Let $y = -x$. Then $dy = -dx$ and

$$\int_{-\pi}^{\pi} f(x)\cos(x)dx = \int_{-\pi}^{\pi} f(-y)\cos(-y)dy = \int_{-\pi}^{\pi} f(-y)\cos(y)dy.$$

  We only need to determine two coefficients

$$\begin{aligned} 0 &= \int_{-\pi}^{\pi} 1\cos(x)dx = 2A_0 + 2A_1, \\ -4\pi &= \int_{-\pi}^{\pi} x^2\cos(x)dx = 2A_0\left(\frac{3}{4}\pi\right)^2 + 2A_1\left(\frac{1}{4}\pi\right)^2. \end{aligned}$$

- Solving the system, we obtain $A_1 = A_2 = -A_0 = -A_3 = 4/\pi$.

$$\int_{-\pi}^{\pi} f(x)\cos(x)dx \approx \frac{4}{\pi}\left\{-f\left(-\frac{3}{4}\pi\right) + f\left(-\frac{1}{4}\pi\right) + f\left(\frac{1}{4}\pi\right) - f\left(\frac{3}{4}\pi\right)\right\}.$$

Exercise

- Find a formula

$$\int_0^1 f(x)e^x dx \approx A_0 f(0) + A_1 f(1)$$

that is exact when f is a polynomial of degree one.

- Verify the formula by computing

$$\int_0^1 (2x+3)e^x dx.$$

(The formula should be exact for this definite integral!)

Change of intervals

- Suppose we have a numerical integration formula for an interval $[c, d]$, can we use it for a problem defined on a different interval $[a, b]$?
- Suppose a formula is given

$$\int_c^d f(t)dt \approx \sum_{i=0}^{n} A_i f(t_i)$$

and we don't know, or care, where the formula comes from.

Change of intervals (cont'd)

- Define a linear function λ that maps the interval $[c, d]$ to another interval $[a, b]$ such that if t traverses $[c, d]$, $\lambda(t)$ will traverse $[a, b]$.
- That means $\lambda(c) = a$ and $\lambda(d) = b$, and λ is given explicitly by

$$\lambda(t) = a\frac{t-d}{c-d} + b\frac{t-c}{d-c} \left(= \frac{b-a}{d-c}t + \frac{ad-bc}{d-c} \right)$$

or

$$x = a\frac{t-d}{c-d} + b\frac{t-c}{d-c}.$$

Change of intervals (cont'd)

- To make the change of variable, we also need to compute dx in terms of dt. Taking the derivative, we have

$$dx = \left(a\frac{1}{c-d} + b\frac{1}{d-c} \right) dt = \frac{b-a}{d-c}dt$$

which implies

$$\int_a^b f(x)dx = \int_c^d f(\lambda(t))\frac{b-a}{d-c}dt.$$

- So we have

$$\int_a^b f(x)dx \approx \frac{b-a}{d-c}\sum_{i=0}^{n} A_i f\left(a\frac{t_i-d}{c-d} + b\frac{t_i-c}{d-c} \right).$$

Exercise

Suppose that we have derived Simpson's rule

$$\int_0^1 f(x)dx \approx \frac{1}{6}f(0) + \frac{2}{3}f(0.5) + \frac{1}{6}f(1)$$

using the method of undermined coefficients. Use the change of intervals to derive a corresponding formula for

$$\int_a^b f(x)dx.$$

(The formula is given on page 25!)

Error analysis

- Recall the interpolation error

$$f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i).$$

Taking the integral, we have

$$\int_a^b f(x)dx - \sum_{i=0}^{n} A_i f(x_i) = \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i) dx,$$

where

$$A_i = \int_a^b \ell_i(x) dx.$$

- If $|f^{(n+1)}(x)| \leq M$ on $[a, b]$, then we have

$$\left| \int_a^b f(x)dx - \sum_{i=0}^{n} A_i f(x_i) \right| \leq \frac{M}{(n+1)!} \int_a^b \prod_{i=0}^{n} |(x - x_i)| dx.$$

Therefore, The accuracy depends on the distribution of the points.

Gaussian quadrature

- The formula

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

is obtained in two steps:

(1) select the nodes $x_0, x_1, \cdots, x_n$

(2) determine A_i so that the formula is exact for polynomials of degree $\leq n$

- **Question:** *since we have $2n+2$ parameters to choose, $x_0, x_1, \cdots, x_n$ and $A_0, A_1, \cdots, A_n$, can we make a formula that is exact for all polynomials of degree $\leq 2n+1$?*

Example

Let us take a two-point case as an example. Consider the interval $[-1,1]$, let us pick two point $x_0, x_1 \in [-1,1]$ such that

$$\int_{-1}^{1} f(x)dx \approx A_0 f(x_0) + A_1 f(x_1)$$

is exact for polynomials of degree ≤ 3. That means the formula produces no error for the functions $1, x, x^2$, and x^3.

$$\begin{aligned} 2 &= \int_{-1}^{1} 1dx = A_0 + A_1, \\ 0 &= \int_{-1}^{1} xdx = x_0 A_0 + x_1 A_1, \\ \frac{2}{3} &= \int_{-1}^{1} x^2 dx = x_0^2 A_0 + x_1^2 A_1, \\ 0 &= \int_{-1}^{1} x^3 dx = x_0^3 A_0 + x_1^3 A_1, \end{aligned}$$

We have four equations and four unknowns, a nonlinear system of equations. *(In general, it is difficult to solve the nonlinear system!)*

Example (cont'd)

- Solution is $A_0 = A_1 = 1$ and $x_1 = -x_0 = 1/\sqrt{3}$.
- The two-point Gaussian formula is:

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

It is exact for polynomials of degree ≤ 3.

Theorem on Gaussian quadrature

Let $w(x)$ be a positive weight function and let $q(x)$ be a nonzero polynomial of degree $n+1$ that is w-orthogonal to the space Π_n in the sense that

$$\int_a^b q(x)p(x)w(x)dx = 0 \quad \textit{for all } p(x) \in \Pi_n.$$

If $x_0, x_1, \cdots, x_n$ are the roots of $q(x) = 0$, then the formula

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

is exact for all $f(x) \in \Pi_{2n+1}$ with $A_i = \int_a^b w(x) \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j} dx.$

Proof. (cf. Textbook, page 493)

$f \in \Pi_{2n+1} \Longrightarrow f = qp + r$ for some $p, r \in \Pi_n \Longrightarrow f(x_i) = r(x_i)$.

$$\therefore \int_a^b fw dx = \int_a^b qpw + rw dx = \int_a^b rw dx \underbrace{=}_{exact} \sum_{i=0}^{n} A_i r(x_i) = \sum_{i=0}^{n} A_i f(x_i). \quad \square$$

How to find $q(x)$?

- **Note:** *It can be proved that the polynomial $q(x)$ only has simple roots and all roots are in $[a, b]$* (cf. Textbook, page 494).

  Proof. $\because 1 \in \Pi_n$, $\int_a^b 1qw\,dx = 0$ and $w > 0$ on $[a, b]$.
  $\therefore q$ changes sign at least once.
  Suppose that q changes sign only r times with $r \le n$. Let $a = t_0 < t_1 < \cdots < t_r < t_{r+1} = b$ and $q(t_i) = 0$, $i = 1, 2, \cdots, r$.
  Then q is of one sign on each $(t_0, t_1), (t_1, t_2), \cdots, (t_r, t_{r+1})$.
  $p(x) := \prod_{i=1}^{r}(x - t_i) \in \Pi_n$ has the same sign property.
  $\therefore \int_a^b qpw\,dx \neq 0$, a contradiction!

- How do we find this $q(x)$? On $[-1, 1]$, $w(x) = 1$,

  Legendre polynomials : $q_n(x) = \dfrac{n!}{(2n)!}\dfrac{d^n((x^2-1)^n)}{dx^n}$.

$$q_1(x) = x, \text{ root: } 0, \quad q_2(x) = x^2 - \frac{1}{3}, \text{ roots: } -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}},$$
$$q_3(x) = x^3 - \frac{3}{5}x, \text{ roots: } -\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}.$$

Convergence and error analysis

- **Theorem:** *If $f(x)$ is continuous, then Gaussian quadrature*

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_{ni} f(x_{ni})$$

converges as $n \to \infty$.

Proof. See page 497 of the textbook.

- **Theorem:** *Gaussian formula with error term is*

$$\int_a^b f(x)w(x)dx = \sum_{i=0}^{n-1} A_i f(x_i) + E.$$

For an $f \in C^{2n}[a,b]$, we have

$$E = \frac{f^{(2n)}(\xi)}{(2n)!} \int_a^b q^2(x)w(x)dx,$$

where $a < \xi < b$ and $q(x) = \prod_{i=0}^{n-1}(x - x_i)$.

Proof. See page 497 of the textbook.