Computational Electromagnetics : Numerical Integration

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Topics in this module

1. Simple Numerical Integration ✓
2. Interpolating a Function ✓
3. Advanced Numerical Integration ✓

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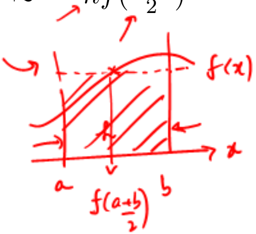
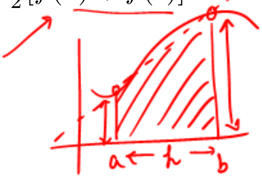
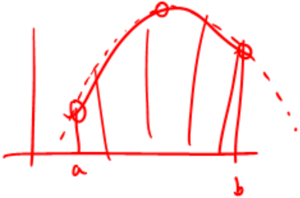
Simple numerical integration

Take a function $f(x)$ that has no analytical integral, want: $\boxed{\int_a^b f(x)\,dx}$

	0	1	2
Rules:	Rectangle	Trapezoidal	Simpson's
$I \approx$	$hf(\frac{a+b}{2})$	$\frac{h}{2}[f(a)+f(b)]$	$\frac{h}{3}[f(a)+4f(\frac{a+b}{2})+f(b)]$







Simple Numerical Integration (contd.)

What was the basis of these simple rules? Taylor's theorem:

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x-x_0)^2}{2} f''(x - x_0) + \cdots$$

$f' \to f'(x_0) = f'(0)$

$x_0 = 0$

$$\left[f(x) = f(0) + x f' + x^2/2 \, f'' + \cdots \right]$$

Now, $\underbrace{\int_0^h f(x)\,dx}_{I} = h f(0) + \left.\frac{x^2}{2}\right]_0^h f' + \left.\frac{x^3}{6}\right]_0^h f'' + \cdots$

$$= h f(0) + \frac{h^2}{2} f' + \frac{h^3}{6} f'' + \cdots$$

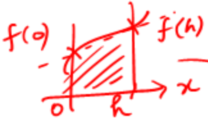
$f'(0) = \frac{f(h) - f(0)}{h}$

Rectangle $\quad I = h f(0) + O(h^2 f')$

Trapezoidal $\quad I = h f(0) + \frac{h^2}{2}\left(\frac{f(h) - f(0)}{h}\right) + O(h^3 f'')$

$$= \frac{h}{2}\left[f(0) + f(h)\right] + O(h^3 f'')$$

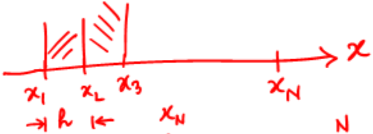
[called Newton-Cotes formulas]



Extended rules – idea of 'quadrature rule'

Extend trapezoidal rule $\int_0^h f(x)\,dx \approx \frac{h}{2}[f(0)+f(h)]$ for $\int_{x_1}^{x_N} f(x)\,dx$

$$= h\left[\frac{1}{2}f(x_1) + f(x_2) + \cdots + \frac{1}{2}f(x_N)\right]$$



$$\int_{x_1}^{x_N} f(x)\,dx = \sum_{i=1}^{N} f(x_i)\, w_i \qquad w_i = \begin{cases} h/2, & i=1,N \\ h & \text{else} \end{cases}$$

$$\int_{x_1}^{x_N} g(x)\,dx = \sum_{i=1}^{N} g(x_i)\, w_i$$

Quadrature rule – a formula in terms of:

∗ weights, ← w_i

∗ function evaluation points ← x_i

'nodes'

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

Interpolating a function

Many functions we want to integrate can't be done analytically.

- What can be done? Weierstrass Approximation Theorem:
  If f is a continuous real-valued function on $[a, b]$ and if any $\epsilon > 0$ is given, then there exists a polynomial p on $[a, b]$ such that $|f(x) - p(x)| < \epsilon$ for all $x \in [a, b]$.
- Fn known at few points – interpolate a polynomial fn: 2, 3, . . . , N

line

parabola

poly order $(N-1)$

x_0, x_1, x_2. $p(x) = a_0 + a_1 x + a_2 x^2$

$p(x_0) = a_0 + a_1 x_0 + a_2 x_0^2$

3 eqns/3 vars

a_0, a_1, a_2 soln

$L_i(x) = \prod_{\substack{j=1 \\ j \neq i}}^{N} \left(\frac{x - x_j}{x_i - x_j} \right)$

$L_i(x_i) = 1$

$L_i(x_j) = 0$, $i \neq j$

const

$\boxed{\text{poly } (N-1)}$

Lagrange polynomials

order $N-1$

$f_{N-1}(x_i) = f(x_i)$

$f_{N-1}(x) = \sum_{i=1}^{N} f(x_i) L_i(x)$

N nodes $x_1, x_2, \cdots, x_N$

Integrating this interpolated function

$$\int_{x_1}^{x_N} f(x)\,dx \approx \int_{x_1}^{x_N} \overset{\text{order } N-1}{f_{N-1}(x)}\,dx = \int_{x_1}^{x_N} \sum_{i=1}^{N} f(x_i) L_i(x)\,dx$$

$$= \sum_{i=1}^{N} f(x_i) \underbrace{\int_{x_1}^{x_N} L_i(x)\,dx}$$

$$= \sum_{i=1}^{N} f(x_i)\, w_i$$

x_i nodes

wts → precomputed.

indep$^{\underline{n}}$ of fn chosen.

Another kind of quadrature rule

Accurate to polynomial order $N-1$, needing N points

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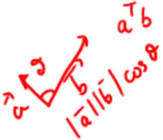
Gauss

Can we do better? Gaussian quadrature

Summary: Clever math gives poly accuracy of order $2N-1$ using N points

0. We know the inner product of vectors ... but functions?



$f(x), g(x) \rightarrow (f,g) = \int_a^b f(x)g(x)\,dx.$

if $(f,g)=0$ then f,g are orthogonal.

1. Construct a polynomial $p_N(x)$ (order N) s.t. $\int_a^b x^k p_N(x)\,dx = 0,\ k \in [0, N-1]$

$1, x, x^2, \quad [-1,1] \qquad f_0(x)=1$

$f_2(x)=x^2$

$$\int_{-1}^{1} f_0(x) f_2(x)\,dx = \int_{-1}^{1} x^2\,dx = \frac{x^3}{3}\Big|_{-1}^{1} = \frac{2}{3}$$

Gram-Schmidt $\rightarrow$ Legendre Polynomials

Gaussian quadrature (contd.)

zeros

2. Roots of $p_N(x)$?

N roots. orthogonal → real, distinct roots.

$P_N(x_i) = 0$

3. Approximate $f(x)$ to poly order $2N-1$ using $p_N(x)$ (Euclidean division)

$$\frac{f_{2N-1}(x)}{p_N(x)} = q(x) + \frac{r(x)}{P_N(x)}$$

q, r : order $< N$.

e.g. $\frac{3x^3-2x^2+4x-3}{x^2+3x+3} = (3x - 11) + \frac{28x+30}{x^2+3x+3}$.

3

2

$$\implies f_{2N-1}(x) = q(x)P_N(x) + r(x)$$

approx to order $2N-1$

Gaussian quadrature (contd.)

4. Now integrate on both sides of: $\int_{x_1}^{x_N} \left(f_{2N-1}(x) = q(x)P_N(x) + r(x) \right) dx$

$$\int \left(\cancel{a_0 + a_1 x + \cdots + a_{N-1} x^{N-1}} \right) P_N(x)\, dx$$

$$\int_{x_1}^{x_N} L_i(x)\, dx$$

$$\hookrightarrow \int_{x_1}^{x_N} f_{2N-1}(x)\, dx = \int_{x_1}^{x_N} r(x)\, dx = \sum_{i=1}^{N} r(x_i)\, w_i$$

Lagrange polynomials for $r(x)$

$$\rightarrow f_{2N-1}(x_i) = 0 + r(x_i) \approx f(x_i)$$

5. If the $\boxed{N \text{ points are chosen as roots of } p_N(x)?}$

$$\int_{x_1}^{x_N} f_{2N-1}(x)\, dx \approx \sum_{i=1}^{N} f(x_i)\, w_i$$

Called Gauss-Lengedre quadrature rule,
accurate to order $2N - 1$.

Gaussian quadrature (contd.)

Take an example, $f(x) = (x+1)^3$ over $[-1, 1]$

$p_0(x) = 1, \quad p_1(x) = x, \quad p_2(x) = (3x^2-1)/2$

$(p_0, p_1) = \int_{-1}^{1} x\,dx = 0$

$(p_0, p_2) = \int_{-1}^{1} \frac{(3x^2-1)}{2}\,dx = \frac{1}{2}\left[\frac{3x^3}{3}\Big|_{-1}^{1} - \frac{x}{2}\Big|_{-1}^{1}\right] = 0$

2-pt Gauss-Lengendre quadrature

$N=2 \quad x_i = \pm\frac{1}{\sqrt{3}}, \; w_i = 1$

$= \sum w_i f(x_i)$

$= 1\times f\left(-\frac{1}{\sqrt{3}}\right) + 1\times f\left(\frac{1}{\sqrt{3}}\right)$

$= \left(1-\frac{1}{\sqrt{3}}\right)^3 + \left(1+\frac{1}{\sqrt{3}}\right)^3$

$= [2]\left[\left(1-\frac{1}{\sqrt{3}}\right)^2 - \left(1-\frac{1}{3}\right) + \left(1+\frac{1}{\sqrt{3}}\right)^2\right]$

$= 4.$ accurate to order $2N-1 = 3.$

Exact calculation $\rightarrow$ $\int_{-1}^{1} f(x)\,dx = \frac{(x+1)^4}{4}\Big|_{-1}^{1} = \frac{2^4}{4} - 0 = 4$

3-pt trapezoidal rule $= 1\times\left[\frac{f(-1)}{2} + f(0) + \frac{f(1)}{2}\right]$

$h=1 \qquad = 1\times\left[0 + 1 + \frac{2^3}{2}\right] = 5$ ✗

Topics that were covered in this module

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Reference: Chapter 4 of Numerical recipes in C++ - Brian P. Flannery, Saul Teukolsky, William H. Press, and William T. Vetterling