Quadrature Examples, Definitions, ETC

We focus on quadrature rules that use a summation like in the following expression.

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

The coefficients $\mathbf{w_i}$ are called the (*quadrature*) ***weights*** and the $\mathbf{x_i}$ are called the **quadrature *points***. The majority of quadrature rules that we consider are linear combinations of values of integrand, but others also incorporate values of its derivative.

Interpolatory Quadrature

If we approximate the integrand **f(x)** using an interpolant **P(x)**, then we can construct a quadrature formula by integrating the interpolant. We call such formulas quadrature of *interpolatory type*. The interpolant **P(x)** can be a polynomial interpolant, a piecewise polynomial interpolant, or even a spline.

A family of quadrature rules known as **Newton-Cotes Formulas** is a constructed by first interpolating the integrand at equispaced points in interval [a, b] and integrating the interpolant. For a set $S = \{(x_i, f(x_i)) \mid i = 0,1,2,...,n\}$ of equispaced points with $x_{i+1} - x_i = h$, to obtain Newton-Cotes formulas we construct the Lagrange interpolant **P(x)**, and then integrate **P(x)**. We get different formulas depending on the number of quadrature points chosen and the location of the points within interval [a, b].

Examples:

Trapezoidal Rule: chose $x_0 = a$ and $x_1 = b$, then the interpolant is a straight line and the resulting Newton-Cotes formula is

$$\int_{x_0}^{x_1} p(x)\,dx = \int_{x_0}^{x_1} \left(\frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \right) dx$$

$$= \frac{x_1 - x_0}{2}\left[f(x_0) + f(x_1)\right] = \frac{h}{2}\left[f(x_0) + f(x_1)\right], \text{ where } h = x_1 - x_0 = b - a$$

Simpson's Rule: chose $x_0 = a$, $x_1 = (a + b)/2$, and $x_2 = b$ then the interpolant is a parabola and the resulting Newton-Cotes formula is

$$\int_{x_0}^{x_2} p(x)\,dx$$

$$= \int_{x_0}^{x_2} \left(\frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \right) dx$$

$$= \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right], \text{ where } h = \frac{b - a}{2}$$

Midpoint Rule: chose $\mathbf{x_0 = (a + b)/2}$ then the interpolant is a horizontal line and the resulting Newton-Cotes formula is

$$\int_a^b \mathbf{p(x)\,dx} = \int_a^b \mathbf{f}\left(\frac{\mathbf{a+b}}{2}\right)\mathbf{dx} = \mathbf{f}\left(\frac{\mathbf{a+b}}{2}\right)(\mathbf{b-a}) = \mathbf{h\ f}\left(\frac{\mathbf{a+b}}{2}\right), \text{ where } \mathbf{h = b - a}$$

The trapezoidal and Simpson's rule are called ***closed*** Newton-Cotes formulas because the end points, a and b, are interpolated. The midpoint rule is called an ***open*** Newton-Cotes formula because neither end point, a nor b, is interpolated. We can generate a variety of both open and closed Newton-Cotes formulas by integrating interpolants constructed from a selection of equispaced points.

Definition
A quadrature formula is said to be of **degree of precision** k if it integrates polynomials of degree k or less exactly, but not polynomials of degree k+1.

Example: Determine the degree of precision of the quadrature formula

$$\int_0^1 f(x)\,dx \approx \frac{9}{4}h\,f(x_1) + \frac{3}{4}h\,f(x_2)$$

where h = 1/3, $x_0 = 0$, $x_1 = 1/3$, $x_2 = 1$.

Note: The objective of degree of precision is to determine the class of polynomials of degree n or less that the quadrature formula will integrate exactly. Since the integral is a linear operator meaning,

$$\int (f(x) + g(x))\,dx = \int f(x)\,dx + \int g(x)\,dx \text{ and } \int kf(x)\,dx = k\int f(x)\,dx,$$

we need only check the behavior of the quadrature formula on a set of basis vectors for the vector space of polynomials. The simplest basis to use is {1, x, x^2, x^3, …, etc.}.

Solution: Simplifying the quadrature formula we get

$$\int_0^1 f(x)\,dx \approx \frac{9}{4}\left(\frac{1}{3}\right) f(1/3) + \frac{3}{4}\left(\frac{1}{3}\right) f(1) = \frac{3}{4} f(1/3) + \frac{1}{4} f(1).$$

Basis function f(x)	$\int_0^1 f(x)\,dx$	Quadrature value $\frac{3}{4} f(1/3) + \frac{1}{4} f(1)$
f(x) = 1	$\int_0^1 1\,dx = 1$	$\frac{3}{4}1 + \frac{1}{4}1 = 1$
f(x) = x	$\int_0^1 x\,dx = \frac{1}{2}$	$\frac{3}{4}\frac{1}{3} + \frac{1}{4}1 = \frac{1}{2}$
f(x) = x^2	$\int_0^1 x^2\,dx = \frac{1}{3}$	$\frac{3}{4}\frac{1}{9} + \frac{1}{4}1 = \frac{1}{3}$
f(x) = x^3	$\int_0^1 x^3\,dx = \frac{1}{4}$	$\frac{3}{4}\frac{1}{27} + \frac{1}{4}1 \neq \frac{1}{4}$

Thus this quadrature formula has degree of precision 2. Hence it will integrate exactly any quadratic polynomial.

Error in the Trapezoidal Rule

Let $h = x_1 - x_0$, then the Error in the Trapezoidal Rule is

$$\textbf{Error(trap)} = -\frac{h^3}{12} f''(\beta) \text{ for } \beta \text{ in } (x_0, x_1).$$ The error is $O(h^3)$.

Example: Approximate the value of $\int_1^3 \frac{1}{x^2}\,dx$ using the Trapezoidal Rule. Compute the absolute error in the approximation and the theoretical error bound. Does the theoretical error "hold"?

Solution: $\int_1^3 \frac{1}{x^2}\,dx = \left[-x^{-1}\right]_1^3 = \frac{2}{3}$ and the Trapezoidal approximation is

$\frac{b-a}{2}[f(a)+f(b)] = \frac{3-1}{2}\left[1+\frac{1}{9}\right] = \frac{10}{9}$ so the absolute error is $\left|\frac{2}{3} - \frac{10}{9}\right| = 0.4444\bar{4}$.

The theoretical error bound is given by

$$\left|\frac{-(b-a)^3}{12} f''(\xi)\right| \le \frac{(b-a)^3}{12} \max_{a \le \xi \le b} |f''(\xi)| = \frac{(2)^3}{12} \max_{1 \le \xi \le 3} \left|\frac{6}{x^4}\right| = \frac{8}{12}\frac{6}{1} = 4.$$

We see that the absolute error is less than the theoretical error as it should be. Theoretical error bounds are by construction pessimistic; in fact worst case scenarios.

A table of closed and open Newton-Cotes formulas, together with their error expressions and degree of precision is displayed next. Carefully inspect the pattern for the degree of precision as more points are used for the interpolant that is integrated.

Closed Newton Cotes Formulas

$$I(f) = \int_a^b f(x)dx \qquad x_0 = a \qquad x_n = b \qquad h = \frac{b-a}{n}$$

n	Formula	Deg. Prec
1	$\frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f^{(2)}(\alpha)$ Trap Rule	1
2	$\frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\alpha)$ Simp 1/3 Rule	3
3	$\frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\alpha)$ Simp 3/8 Rule	3
4	$\frac{2h}{45}[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] - \frac{8h^7}{945} f^{(6)}(\alpha)$	5
5	$\frac{5h}{288}[19f(x_0) + 75f(x_1) + 50f(x_2) + 50f(x_3) + 75f(x_4) + 19f(x_5)] - \frac{275h^7}{12096} f^{(6)}(\alpha)$	5

Open Newton Cotes Formulas

$$I(f)=\int_a^b f(x)dx \qquad x_0=a+h \qquad x_n=b-h \qquad h=\frac{b-a}{n+2}$$

n	Formula	Deg. Prec
0	$2hf(x_0)+\frac{h^3}{3}f^{(2)}(\alpha)$ Midpoint Formula	1
1	$\frac{3h}{2}[f(x_0)+f(x_1)]+\frac{h^3}{4}f^{(2)}(\alpha)$	1
2	$\frac{4h}{3}[2f(x_0)-f(x_1)+2f(x_2)]+\frac{28h^5}{90}f^{(4)}(\alpha)$	3
3	$\frac{5h}{24}[11f(x_0)+f(x_1)+f(x_2)+11f(x_3)]+\frac{95h^5}{144}f^{(4)}(\alpha)$	3
4	$\frac{6h}{20}[11f(x_0)-14f(x_1)+26f(x_2)-14f(x_3)+11f(x_4)]+\frac{41h^7}{140}f^{(6)}(\alpha)$	5

Newton-Cotes formulas derived from the integration of high degree interpolants are rarely used in practice. The reason for this is related to the "polynomial wiggle" problem. (Explain!) Most approximations using Newton-Cotes formulas use a **composite formulation** of these basic formulas.

The composite formulations give us **Riemann sums**. As we increase n, the number of subintervals, and require that the maximum length of the subintervals converges to zero, the limit of the Riemann sums converges to the value of the integral, assuming the integrand is continuous on the interval of integration. In contrast, if we construct a sequence of approximations using Newton-Cotes formulas of increasing degree of precision, this sequence of approximations is not guaranteed to converge to the value of the integral. See the next example.

Example: We have $\int_4^{-4}\frac{\mathbf{dx}}{1+\mathbf{x}^2}=2\,\mathbf{arctan(4)}\approx 2.6516353$.
The following table displays the approximations generated by Newton-Cotes formulas with increasing degree of precision.

Degree of Precision	Approximation from the Closed Newton Cotes Formula
3	5.490
5	2.278
7	3.329
9	1.941
11	3.596

Continuing to increase the degree of precision actually gives increasingly less accurate result. This behavior result from using high degree polynomial interpolants at equispaced points and is due to the "polynomial wiggle" problem.

The **composite Trapezoidal Rule** is $\frac{h}{2}\left[f(x_0)+2f(x_1)+2f(x_2)+\cdots+2f(x_{n-1})+f(x_n)\right]$

The error in the composite trapezoidal rule is the sum of the errors in each of the standard trapezoidal rule applications over the equispaced intervals. It can be shown that this error can be expressed in the form

$\textbf{Error(composite trap)} = -\frac{x_n - x_0}{12}h^2 f''(\beta)$ for β in (a,b). The error is **O(h²)**, where $h=\frac{b-a}{n}$ and the **rate of convergence** is **O(h²).**

The **composite Simpson's rule** is $\frac{h}{3}\sum_{i=1}^{n/2}\left(f(x_{2i-2}+4f(x_{2i-1})+f(x_{2i})\right)$

$\textbf{Error(composite Simpson's rule)} = -\frac{b-a}{180}h^4 f^{(4)}(\beta)$ for β in (a,b). The error is **O(h⁴)** where $h=\frac{b-a}{n}$ and the **rate of convergence** is **O(h⁴)** .

The **composite Midpoint rule** is

$$h\left[f(x_0+h/2)+f(x_1+h/2)+\cdots+f(x_{n-1}+h/2)\right]=h\sum_{i=0}^{n-1}f\left(x_i+h/2\right)$$

$\textbf{Error(composite midpoint rule)} = \frac{b-a}{24}h^2 f''(\beta)$ for β in (a,b). The error is **O(h²)** where $h=\frac{b-a}{n}$ and the **rate of convergence** is **O(h²)**.

<u>Example:</u> In a previous example we considered the integral

$$\int_4^{-4}\frac{dx}{1+x^2}=2\arctan(4)\approx 2.6516353.$$

Approximations generated by Newton-Cotes formulas with increasing degree of precision did **not** generate a sequence of values converging to the true value of the integral. Here we approximate the integral using composite quadrature. Note that the sequences of approximations in the table indicate convergence to the true value. Explain why.

$h=\frac{b-a}{2^n}$ a = -4, b = 4 values of n	Composite Trapezoidal Rule	Composite Simpson's Rule
1	4.23529411764706	2.47843137254902
2	2.91764705882353	2.57254901960784
3	2.65882352941176	2.64773456352162
4	2.65050680499416	2.65162728295638
5	2.65134716346583	2.65163528066308
6	2.65156325136377	2.65163532441487
7	2.6516173061521	2.6516353271534
8	2.65163082190308	2.65163532732465
9	2.65163420096925	2.65163532733535
10	2.65163504574383	2.65163532733602

Numerical Verification of Rates of Convergence

When we know the exact solution we can check the order of convergence as follows. If $\mathbf{e_h}$ is the absolute error using stepsize h, then inspecting the sequence of ratios $\frac{e_h}{e_{h/2}}$ as h → 0 we should see that this sequence converges to 4 when the quadrature formula rate of convergence $\mathbf{O(h^2)}$ (as in the Trapezoidal rule) and this sequence should converge to 16 when the rate of convergence $\mathbf{O(h^4)}$ (as in Simpson's rule).

We can still numerically verify a rate of convergence **when the exact solution is not known**, we just need to examine a different ratio. Let $\mathbf{C_h(f)}$, $\mathbf{C_{h/2}(f)}$, and $\mathbf{C_{h/4}(f)}$ denote composite quadrature approximations obtained by using subintervals of size h, h/2 and h/4 respectively. Consider the ratio

$$\frac{C_h(f) - C_{h/2}(f)}{C_{h/2}(f) - C_{h/4}(f)}.$$

Let the exact value of the integral be denoted by $\mathbf{I(f)}$ and let $e_h = C_h(f) - I(f)$ which is the error associated with the quadrature approximation $\mathbf{C_h(f)}$. Note that if we add zero in disguise to the numerator and denominator of

$$\frac{C_h(f) - C_{h/2}(f)}{C_{h/2}(f) - C_{h/4}(f)}$$

in the form $\mathbf{-I(f) + I(f)}$ we obtain

$$\frac{C_h(f) - I(f) + I(f) - C_{h/2}(f)}{C_{h/2}(f) - I(f) + I(f) - C_{h/4}(f)} = \frac{e_h - e_{h/2}}{e_{h/2} - e_{h/4}}.$$

If the rate of convergence is k, then $e_h \approx k\, e_{h/2}$, hence we have

$$\frac{C_h(f) - I(f) + I(f) - C_{h/2}(f)}{C_{h/2}(f) - I(f) + I(f) - C_{h/4}(f)} = \frac{e_h - e_{h/2}}{e_{h/2} - e_{h/4}} \approx \frac{k\, e_{h/2} - e_{h/2}}{e_{h/2} - \frac{1}{k} e_{h/2}} = k$$

for sufficiently small h.

Example: For $\int_{4}^{-4} \frac{dx}{1+x^2} = 2\arctan(4)$ we had the Trapezoidal approximations shown in the table. Replace C in the preceding development by T (for Trapezoidal rule) and compute $\frac{T_h(f) - T_{h/2}(f)}{T_{h/2}(f) - T_{h/4}(f)}$ from the data. We get rounded to 4 places ➔

5.0909
31.121
-9.8966
3.889
3.9976
3.9994
3.9998
4

$h = \frac{b-a}{2^n}$ a = -4, b = 4 values of n	Composite Trapezoidal Rule
1	4.23529411764706
2	2.91764705882353
3	2.65882352941176
4	2.65050680499416
5	2.65134716346583
6	2.65156325136377
7	2.6516173061521
8	2.65163082190308
9	2.65163420096925
10	2.65163504574383

Another type of problem is to determine the spacing h required for a specified accuracy in a quadrature formula. We illustrate this in the next example.

Example: Determine the spacing h needed for the composite trapezoidal rule to approximate $\int_0^2 \frac{1}{x+4}\,dx$ so that the error is less than or equal to 10^{-5}.

Using the error term for the composite trapezoidal rule we have

$$|error| = \left|\frac{b-a}{12}h^2 f''(\alpha)\right| = \frac{2-0}{12}h^2\left|\frac{2}{(\alpha+4)^3}\right| \le \frac{1}{6}h^2 \max_{x\in[0,2]}\left|\frac{2}{(x+4)^3}\right|$$

Since $\frac{2}{(x+4)^3}$ is monotonically decreasing on [0, 2] the maximum is at x = 0. Thus we have

$$|error| \le \frac{1}{6}h^2 \max_{x\in[0,2]}\left|\frac{2}{(x+4)^3}\right| \le \frac{1}{6}h^2\frac{2}{4^3} = \frac{h^2}{192}$$

Next we determine h so that $\frac{h^2}{192} \le 10^{-5}$. It follows that $h^2 \le 192 * 10^{-5}$ so $h < 0.0438$. Lets chose h = 0.043 (a bit smaller to ensure the desired accuracy), then for the composite trapezoidal rule $n = \frac{b-a}{h} = \frac{2}{0.043} \approx 46.51$. Thus we need to round up and so we take n = 47. Using the composite trapezoidal rule with n = 47 we get $\int_0^2 \frac{1}{x+4}\,dx \approx 0.405470347$. Comparing this approximation to the true value of the integral which is $\ln(6) - \ln(4) \approx 0.405465108$ we get $|0.405465108 - 0.405470347| \approx 0.000005 = 5 * 10^{-6}$.

MATLAB Routines

The m-files **trap**, **simp**, and **midpt** compute the composite rules respectively for the Trapezoidal, Simpson's and midpoint approximations. Read the help files to understand how to structure the input.

Example: To illustrate the use of the midpoint formula, an open Newton-Cotes rule, we estimate the value of the integral $\int_0^1 \frac{dx}{\sqrt{x}}$.

The integrand is not defined at x = 0, so a closed Newton-Cotes formula is not applicable. (At x = 0 the integral is said to have an *endpoint singularity*.) The behavior of the integrand near x = 0 makes this a challenging problem for the composite midpoint rule. We use MATLAB routine **midpt** for the computations. The exact value of the integral is 2, so we can compute the relative error in our approximations.

```
f='1/sqrt(x)';
format long g
data=[];
for k=0:10
        n=2^k;
        v=midpt(f,0,1,n);
        RE=(2-v)/2;
        data=[data;[n v,RE]];
end
data
```

n	midpt approx	Relative Error
1	1.41421356237309	0.292893218813453
2	1.57735026918963	0.211324865405187
4	1.69884407957967	0.150577960210164
8	1.78646100173484	0.106769499132579
16	1.84885668463974	0.0755716576801311
32	1.89308835970638	0.0534558201468083
64	1.92439275569951	0.0378036221502436
128	1.94653527997052	0.0267323600147399
256	1.96219415267706	0.0189029236614721
512	1.97326708367945	0.0133664581602736
1024	1.98109693726129	0.00945153136935595

The slow convergence of the midpoint formula is due to the singularity in $f(x) = \frac{1}{\sqrt{x}}$ at x = 0. The magnitude of the derivative of f(x) increases without bound as x approaches 0. The midpoint rule consistently under estimates the contribution to the integral that occurs to the left of the first midpoint in the algorithm.