CME 108/MATH 114
Introduction to Scientific Computing
Instructor: Willie Aboumrad
Summer 2020

Notes on Newton-Cotes quadrature

We begin by noting that a quadrature rule is an approximation of the form

$$\int_a^b f(x)dx \approx \sum_j w_j f_j,$$

where $f_j = f(x_j)$ and the sum is taken over a finite index. Therefore, to specify a quadrature, we must provide a list of points (formally termed abscissas) $x_i \in [a, b]$ and a set of weights w_j.

Remark. This problem is analogous to the numerical differentiation problem we just discussed. In that case, we sought coefficients α_j such that

$$f'(x_i) \approx \sum_j \alpha_j f_j.$$

Since the problems are so similar, we will in fact approach them the same way (at first).

First we discuss the general non-composite Newton-Cotes (NC) quadrature rule. This rule is based on polynomial interpolation. To define it, we choose $n + 1$ points in $[a, b]$ as our nodes x_j, and then integrate the corresponding Lagrange basis polynomials $L_{n,j}(x)$ to produce the weights w_j.

Remark. This is exactly analogous to what we did when studying finite differences!

In that case we used

$$f'(x) \approx p'(x)$$

In this case we'll use

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

For simplicity, we typically choose evenly-spaced points, so that $x_{i+1} - x_i = h$, for all i and some $h > 0$. There are two classes of NC rules, corresponding to different placements of x_0 in $[a, b]$. The *closed* NC formulas use the endpoints a, and b as the first and last points. Thus, for these rules we take $h = (b-a)/n$ and choose our points to be $x_i = a + ih$, for $i = 0, 1, \ldots, n$.

The *open* NC rules do not include the endpoints of the interval but they place the first and last point so that they are also at a distance h from the endpoints. Therefore, in this case we take $h = (b-a)/(n+2)$ and choose $x_i = a + (i+1)h$, for $i = 0, 1, \ldots, n$.

In any case, as mentioned above, we derive the weights for the NC rules via polynomial interpolation:

$$\begin{aligned} \int_a^b f(x)dx &\approx \int_a^b p(x)dx \\ &= \int_a^b \sum_{j=0}^n f_j L_{n,j}(x)dx \\ &= \sum_{j=0}^n \left(\int_a^b L_{n,j}(x)dx \right) f_j \\ &= \sum_j w_j f_j, \end{aligned}$$

where the second equality follows by linearity of the integral, with $w_j = \int_a^b L_{n,j}(x)dx$.
Remark. This conclusion is exactly analogous to that in the finite difference case.

In that case we obtained

$$f'(x_i) \approx p'(x_i) = \sum_{j=0}^n d_{ij} f_j,$$

with $d_{ij} = L'_{n,j}(x_i)$.

In this case we conclude

$$\int_a^b f(x)dx \approx \int_a^b p(x)dx = \sum_{j=0}^n w_j f_j,$$

with $w_j = \int_a^b L_{n,j}(x)dx$.

So in both cases we approximate the desired quantity by a weighted sum of function values, and performing the appropriate operation on the Lagrange basis polynomials gives us the right weight.

Given this, in order to specify an NC quadrature we must:

- Decide whether it is open or closed
- Determine $n+1$, the number of points (abscissas)
- Compute $w_j = \int_a^b L_{n,j}(x)dx$, where $L_{n,j}$ denotes the jth Lagrange basis polynomial.

In practical settings, the substitution $x = a + th$ greatly simplifies the weights computation. For example, consider the closed NC rule with $n = 2$. In this case $h = (b-a)/2$ and the three nodes are $x_0 = a$, $x_1 = a + h = (a+b)/2$, and $x_2 = a + 2h = b$. Therefore, the weights are given by

$$
\begin{aligned}
w_0 &= \int_a^b L_{2,0}(x)dx = \int_a^b \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}dx \\
&= \frac{h}{2}\int_0^2 (t-1)(t-2)dt \\
&= \frac{h}{2}\left(\frac{t^3}{3} - \frac{3}{2}t^2 + 2t\bigg|_{t=2}\right) \\
&= \frac{h}{3}, \\
w_1 &= \int_a^b L_{2,1}(x)dx = \int_a^b \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_0-x_2)}dx \\
&= -h\int_0^2 t(t-2)dt \\
&= -h\left(\frac{t^3}{3} - t^2\bigg|_{x=2}\right) \\
&= \frac{4h}{3}, \text{ and} \\
w_2 &= \int_a^b L_{2,2}(x)dx = \int_a^b \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx \\
&= \frac{h}{2}\int_0^2 t(t-1)dt \\
&= \left(\frac{t^3}{3} - \frac{t^2}{2}\bigg|_{t=2}\right) \\
&= \frac{h}{3}.
\end{aligned}
$$

In this case the NC rule simplifies to the familiar Simpson's rule from calculus (see below):

$$\int_a^b f(x)dx \approx \frac{h}{3}\left[f(a) + f\left(\frac{a+b}{2}\right) + f(b)\right].$$

Remark. You may perhaps remember that Simpson's rule is derived by finding the area under the quadratic passing through the points $(a, f(a)), ((a+b)/2, f((a+b)/2)), (b, f(b))$. This is the quadratic which interpolates f at the mid- and endpoints of the interval, and by our uniqueness result this is exactly $\sum_j f_j L_{n,j}(x)$! (The Lagrange basis simply gives us another way of looking at the same quadratic.)

Analogous comments apply to the trapezoidal rule, and we see that the NC rules generalize the integration rules we've seen before.

For completeness, we provide below formulas for some commonly used NC quadrature rules.

We begin with four closed rules.

- The case $n+1 = 1$ yields the **left endpoint** rule. The corresponding quadrature is simply $\int_a^b f(x)dx \approx (b-a)f(a)$.
- The case $n+1 = 2$ yields the **trapezoidal** rule. The corresponding quadrature is $\int_a^b f(x)dx = \frac{b-a}{2}(f(a) + f(b)) - \frac{(b-a)^3}{12} f''(\xi)$, for some $\xi \in [a, b]$.
- The case $n+1 = 3$ yields **Simpson's** rule. The corresponding quadrature is $\int_a^b f(x)dx = \frac{b-a}{6}(f(a) + 4f(\frac{a+b}{2}) + f(b)) - \frac{(b-a)^5}{2880} f^{(4)}(\xi)$, for some $\xi \in [a, b]$.
- Finally, the case $n+1 = 4$ yields the *three-eights* rule. The corresponding quadrature is $\int_a^b f(x)dx \approx \frac{b-a}{8}(f(a) + 3f(a+h) + 3f(a+2h) + f(b))$.

Next, we provide formulas for three open rules.

- The case $n+1 = 1$ yields the **midpoint** rule. The corresponding quadrature is simply $\int_a^b f(x)dx = (b-a)f(\frac{a+b}{2}) + \frac{(b-a)^3}{24} f''(\xi)$, for some $\xi \in [a, b]$.
- In the case $n+1 = 2$ the corresponding quadrature is $\int_a^b f(x)dx = \frac{b-a}{2}(f(a+h) + f(a+2h)) + \frac{(b-a)^3}{36} f''(\xi)$, for some $\xi \in [a, b]$.
- In the case $n+1 = 3$ the corresponding quadrature is $\int_a^b f(x)dx \approx \frac{b-a}{3}(2f(a+h) - f(a+2h) + 2f(a+3h))$.

To conclude, we comment on the degree of precision of the NC quadratures. The *degree of precision* (DOP) of a quadrature rule is the largest integer k such that

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

for every polynomial $p(x)$ of degree at most k. That is, the DOP of a quadrature is the largest integer k such that the quadrature can integrate all polynomials of degree at most k **exactly**: for these p, the quadrature rule gives the exact value of the integral.

As stated precisely in the theorem on page 464 of the textbook, the DOP of the NC quadrature (open or closed) with $n+1$ abscissas is $n+1$ if n is even and n otherwise.

Lastly, when n is even, there exists a $\xi \in [a,b]$ such that the absolute error is proportional to $(b-a)^{n+3} f^{(n+2)}(\xi)$ and when n is odd, there exists a $\xi' \in [a,b]$ such that the error is proportional to $(b-a)^{n+2} f^{(n+1)}(\xi')$.

Finally, we move to composite NC quadratures. Composite NC rules are derived from non-composite rules simply by partitioning the interval of interest $[a,b]$ into a number of subintervals applying the non-composite rule on each subinterval and then summing the results.

For completeness, we provide a couple formulas for composite NC quadrature rules.

- The **composite trapezoidal** rule is given by

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

  for some $\xi \in [a,b]$, with $h = (b-a)/n$ and $x_j = a + jh$.

- The **composite Simpson's** rule is given by

  $$\int_a^b f(x)dx = \frac{h}{3}\left(f(a) + 4\sum_{j=1}^{m} f(x_{2j-1}) + 2\sum_{j=1}^{m-1} f(x_{2j}) + f(b)\right) - \frac{(b-a)h^4}{180} f^{(4)}(\xi),$$

  for some $\xi \in [a,b]$, with $n = 2m$, $h = (b-a)/n$ and $x_j = a + jh$.

Note that whereas the composite trapezoidal rule has rate of convergence $O(h^2)$, the composite Simpson's rule has rate $O(h^4)$.