Newton–Cotes quadrature

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Consider the approximation of $I(f) := \int_a^b f(x)\,dx$ for integrable $f : [a,b] \to \mathbb{R}$ by a **quadrature formula** of the form $I_n(f) := \sum_{j=0}^n w_j f(x_j)$, where $\{w_j\}_{j=0}^n \subseteq \mathbb{R}$ are **weights** and $\{x_j\}_{j=0}^n \subseteq [a,b]$ are *distinct* **nodes**.

The **precision** of a quadrature formula is the greatest m for which $I_n = I$ on P_m (the vector space of real polynomial functions of degree *at most* m). For such an m to exist, we assume that $\sum_{j=0}^n w_j = I_n(1) = I(1) = b - a$ so that $I_n = I$ on P_0 by linearity, while also noting that $m \leq 2n+1$ since $I_n(\omega_{n+1}^2) = 0 < I(\omega_{n+1}^2)$ for $\omega_{n+1} := \prod_{j=0}^n (\bullet - x_j) \in P_{n+1}$. In addition, Lagrange interpolation shows that $m \geq n$ if and only if $I_n(f) = I(p_n)$ for all f, where $p_n \in P_n$ interpolates f at the nodes; or equivalently, $w_j = I(\ell_j)$ for all j, where $\{\ell_j\}_{j=0}^n$ is the Lagrange basis of P_n. Such a formula is called **interpolatory** and its error can be expressed as

$$I(f) - I_n(f) = I(f - p_n) = \int_a^b f[x_0, \ldots, x_n, x]\omega_{n+1}(x)\,dx.$$

Closed Newton–Cotes formulas

For $n \geq 1$, the $(n+1)$-point **closed Newton–Cotes formula** is the interpolatory quadrature formula with $x_j := a + jh$, where $h := \frac{b-a}{n}$.

To analyze its error, we define the polynomials $\Omega_j(x) := \int_a^x \omega_j(t)\,dt$ for $1 \leq j \leq n+1$. We claim that $\Omega_j \geq 0$ or $\Omega_j \leq 0$ on $[a, x_{j-1}]$ according as j is odd or even. This claim is trivial for $j = 1$, and if it holds for some j, integration by parts gives $\Omega_{j+1}(x) = \Omega_j(x)(x - x_j) - \int_a^x \Omega_j(t)\,dt$, which implies that the desired inequality for Ω_{j+1} holds on $[a, x_{j-1}]$. Furthermore, Ω_{j+1} is decreasing on $[x_{j-1}, x_j]$, so if j is odd, then $\Omega_{j+1}(x) \leq \Omega_{j+1}(x_{j-1}) \leq 0$ for all $x \in [x_{j-1}, x_j]$, whereas if j is even, then $\Omega_{j+1}(x) \geq \Omega_{j+1}(x_j) = 0$ for all $x \in [x_{j-1}, x_j]$ by the symmetry of ω_{j+1}, which establishes the claim by induction.

In fact, if j is odd, then $\Omega_j \geq 0$ everywhere because Ω_j is decreasing on $(-\infty, a]$ and increasing on $[x_{j-1}, \infty)$. We also note that $\int_a^b \Omega_j(x)\,dx = -\int_a^b (t-b)\omega_j(t)\,dt$ for all j.

Now if n is even and $f \in C^{n+2}([a,b])$, integration by parts and the mean value theorems for integrals and divided differences yield

$$\begin{aligned}\int_a^b f[x_0, \ldots, x_n, x]\omega_{n+1}(x)\,dx &= -\int_a^b f[x_0, \ldots, x_n, x, x]\Omega_{n+1}(x)\,dx \\ &= -\frac{f^{(n+2)}(\xi)}{(n+2)!}\int_a^b \Omega_{n+1}(x)\,dx \quad \text{for some } \xi \in (a,b) \\ &= \frac{f^{(n+2)}(\xi)}{(n+2)!}\int_a^b t\omega_{n+1}(t)\,dt.\end{aligned}$$

If n is odd and $f \in C^{n+1}([a,b])$, we have

$$\begin{aligned}\int_a^b f[x_0,\dots,x_n,x]\omega_{n+1}(x)\,dx &= \int_a^b \big(f[x_0,\dots,x_{n-1},x]-f[x_0,\dots,x_n]\big)\omega_n(x)\,dx\\ &= -\int_a^b f[x_0,\dots,x_{n-1},x,x]\Omega_n(x)\,dx\\ &= -\frac{f^{(n+1)}(\xi)}{(n+1)!}\int_a^b \Omega_n(x)\,dx \quad \text{for some } \xi\in(a,b)\\ &= \frac{f^{(n+1)}(\xi)}{(n+1)!}\int_a^b \omega_{n+1}(t)\,dt.\end{aligned}$$

In summary, we obtain the following (where we have changed variables affinely to exhibit the dependence of the error and the weights on h).

> **Error of closed Newton–Cotes formulas**
>
> If n is even and $f\in C^{n+2}([a,b])$, then there exists a $\xi\in(a,b)$ such that
>
> $$I(f)-I_n(f)=C_n f^{(n+2)}(\xi)h^{n+3},\quad C_n:=\frac{1}{(n+2)!}\int_0^n x^2(x-1)\cdots(x-n)\,dx.$$
>
> If n is odd and $f\in C^{n+1}([a,b])$, then there exists a $\xi\in(a,b)$ such that
>
> $$I(f)-I_n(f)=C_n f^{(n+1)}(\xi)h^{n+2},\quad C_n:=\frac{1}{(n+1)!}\int_0^n x(x-1)\cdots(x-n)\,dx.$$

n	w_j/h	C_n
1 (**trapezoidal rule**)	$\frac{1}{2},\frac{1}{2}$	$-\frac{1}{12}$
2 (**Simpson's rule**)	$\frac{1}{3},\frac{4}{3},\frac{1}{3}$	$-\frac{1}{90}$
3 (**Simpson's 3/8 rule**)	$\frac{3}{8},\frac{9}{8},\frac{9}{8},\frac{3}{8}$	$-\frac{3}{80}$
4 (**Boole's rule**)	$\frac{14}{45},\frac{64}{45},\frac{8}{15},\frac{64}{45},\frac{14}{45}$	$-\frac{8}{945}$

Open Newton–Cotes formulas

For $n\ge 0$, the $(n+1)$-point **open Newton–Cotes formula** is the interpolatory quadrature formula with $x_j:=a+(j+1)h$, where $h:=\frac{b-a}{n+2}$.

As above, we define $\Omega_j(x):=\int_a^x \omega_j(t)\,dt$ for $0\le j\le n+1$; an analogous argument shows that $\Omega_j\ge 0$ or $\Omega_j\le 0$ on $[a,x_j]$ according as j is even or odd, where $x_{n+1}:=b$. Thus, if n is even and $f\in C^{n+2}([a,b])$, the same argument as before yields

$$\int_a^b f[x_0,\dots,x_n,x]\omega_{n+1}(x)\,dx=\frac{f^{(n+2)}(\xi)}{(n+2)!}\int_a^b t\omega_{n+1}(t)\,dt \quad \text{for some } \xi\in(a,b).$$

However, if n is odd and $f\in C^{n+1}([a,b])$, then Ω_n changes sign at $x_n=b-h$, so the mean value theorem for integrals is not applicable on $[a,b]$ as before. Instead, we write

$$\begin{aligned}\int_a^b f[x_0,\dots,x_n,x]\omega_{n+1}(x)\,dx &= \int_a^{x_n} f[x_0,\dots,x_n,x]\omega_{n+1}(x)\,dx + \int_{x_n}^b f[x_0,\dots,x_n,x]\omega_{n+1}(x)\,dx \\ &= \frac{f^{(n+1)}(\xi_1)}{(n+1)!}\int_a^{x_n}\omega_{n+1}(x)\,dx + \frac{f^{(n+1)}(\xi_2)}{(n+1)!}\int_{x_n}^b \omega_{n+1}(x)\,dx \\ &\text{for some } \xi_1,\xi_2\in(a,b).\end{aligned}$$

Since $\int_a^{x_n}\omega_{n+1}(x)\,dx = \Omega_{n+1}(x_n) \geq 0$ and $\int_{x_n}^b \omega_{n+1}(x)\,dx \geq 0$, the intermediate value theorem implies that this sum is equal to

$$\frac{f^{(n+1)}(\xi)}{(n+1)!}\left(\int_a^{x_n}\omega_{n+1}(x)\,dx + \int_{x_n}^b \omega_{n+1}(x)\,dx\right) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\int_a^b \omega_{n+1}(x)\,dx \quad \text{for some } \xi\in(a,b).$$

> **Error of open Newton–Cotes formulas**
>
> If n is even and $f \in C^{n+2}([a,b])$, then there exists a $\xi \in (a,b)$ such that
>
> $$I(f) - I_n(f) = C_n f^{(n+2)}(\xi)h^{n+3}, \quad C_n := \frac{1}{(n+2)!}\int_{-1}^{n+1} x^2(x-1)\cdots(x-n)\,dx.$$
>
> If n is odd and $f \in C^{n+1}([a,b])$, then there exists a $\xi \in (a,b)$ such that
>
> $$I(f) - I_n(f) = C_n f^{(n+1)}(\xi)h^{n+2}, \quad C_n := \frac{1}{(n+1)!}\int_{-1}^{n+1} x(x-1)\cdots(x-n)\,dx.$$

n	w_j/h	C_n
0 (**midpoint rule**)	2	$\frac{1}{3}$
1	$\frac{3}{2}, \frac{3}{2}$	$\frac{3}{4}$
2	$\frac{8}{3}, -\frac{4}{3}, \frac{8}{3}$	$\frac{14}{45}$
3	$\frac{55}{24}, \frac{5}{24}, \frac{5}{24}, \frac{55}{24}$	$\frac{95}{144}$