Newton-Cotes Formulas

7.1 Introduction to Quadrature

We now approach the subject of numerical integration. The goal is to approximate the definite integral of $f(x)$ over the interval $[a, b]$ by evaluating $f(x)$ at a finite number of sample points.

Definition 7.1. Suppose that $a = x_0 < x_1 < \cdots < x_M = b$. A formula of the form

$$Q[f] = \sum_{k=0}^{M} w_k f(x_k) = w_0 f(x_0) + w_1 f(x_1) + \cdots + w_M f(x_M) \tag{1}$$

with the property that

$$\int_a^b f(x)\,dx = Q[f] + E[f] \tag{2}$$

is called a numerical integration or ***quadrature*** formula. The term $E[f]$ is called the ***truncation error*** for integration. The values $\{x_k\}_{k=0}^{M}$ are called the ***quadrature nodes***, and $\{w_k\}_{k=0}^{M}$ are called the ***weights***. ▲

Depending on the application, the nodes $\{x_k\}$ are chosen in various ways. For the trapezoidal rule, Simpson's rule, and Boole's rule, the nodes are chosen to be equally spaced. For Gauss-Legendre quadrature, the nodes are chosen to be zeros of certain Legendre polynomials. When the integration formula is used to develop a predictor formula for differential equations, all the nodes are chosen less than b. For all applications, it is necessary to know something about the accuracy of the numerical solution.

Definition 7.2. The ***degree of precision*** of a quadrature formula is the positive integer n such that $E[P_i] = 0$ for all polynomials $P_i(x)$ of degree $i \le n$, but for which $E[P_{n+1}] \ne 0$ for some polynomial $P_{n+1}(x)$ of degree $n + 1$. ▲

The form of $E[P_i]$ can be anticipated by studying what happens when $f(x)$ is a polynomial. Consider the arbitrary polynomial

$$P_i(x) = a_i x^i + a_{i-1}x^{i-1} + \cdots + a_1 x + a_0$$

of degree i. If $i \le n$, then $P_i^{(n+1)}(x) \equiv 0$ for all x, and $P_{n+1}^{(n+1)}(x) = (n+1)!a_{n-1}$ for all x. Thus it is not surprising that the general form for the truncation error term is

$$E[f] = Kf^{(n+1)}(c), \tag{3}$$

where K is a suitably chosen constant and n is the degree of precision. The proof of this general result can be found in advanced books on numerical integration.

The derivation of quadrature formulas is sometimes based on polynomial interpolation. Recall that there exists a unique polynomial $P_M(x)$ of degree $\le M$ passing through the $M + 1$ equally spaced points $\{(x_k, f(x_k))\}_{k=0}^{M}$. When this polynomial is used to approximate $f(x)$ over $[a, b]$, and then the integral of $f(x)$ is approximated by the integral of $P_M(x)$, the resulting formula is called a ***Newton-Cotes quadrature formula*** (see Figure 7.2). When the sample points $x_0 = a$ and $x_M = b$ are used, it is called a ***closed*** Newton-Cotes formula. The next result gives the formulas when approximating polynomials of degree $M = 1, 2, 3,$ and 4 are used.

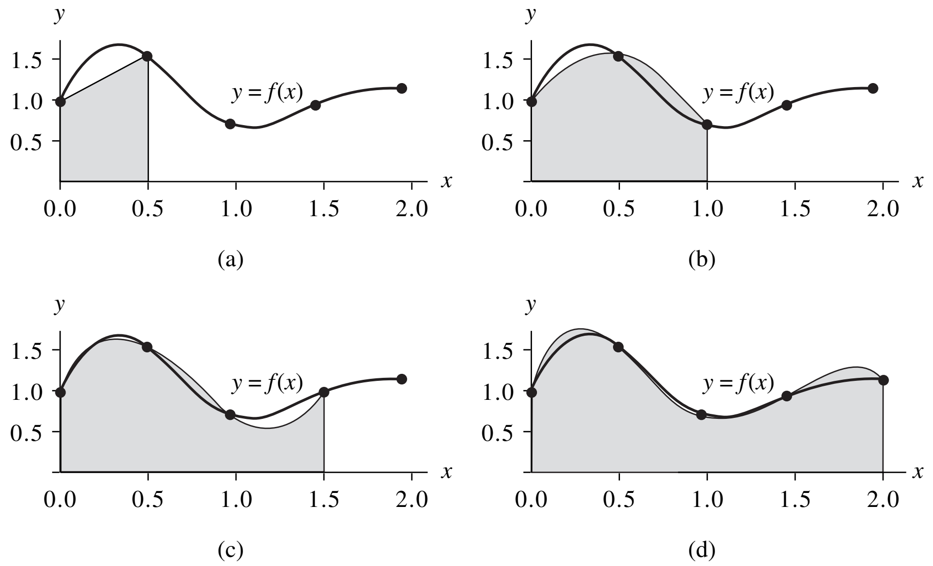
Theorem 7.1 (Closed Newton-Cotes Quadrature Formula). Assume that $x_k = x_0 + kh$ are equally spaced nodes and $f_k = f(x_k)$. The first four closed Newton-Cotes quadrature formulas are

$$\int_{x_0}^{x_1} f(x)\,dx \approx \frac{h}{2}(f_0 + f_1) \qquad \text{(trapezoidal rule)}, \tag{4}$$

$$\int_{x_0}^{x_2} f(x)\,dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2) \qquad \text{(Simpson's rule)}, \tag{5}$$

$$\int_{x_0}^{x_3} f(x)\,dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) \qquad \text{(Simpson's } \tfrac{3}{8} \text{ rule)}, \tag{6}$$

$$\int_{x_0}^{x_4} f(x)\,dx \approx \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) \qquad \text{(Boole's rule)}. \tag{7}$$



(a) (b) (c) (d)

Figure 7.2 (a) The trapezoidal rule integrates $y = P_1(x)$ over $[x_0, x_1] = [0.0, 0.5]$. (b) Simpson's rule integrates $y = P_2(x)$ over $[x_0, x_1] = [0.0, 1.0]$. (c) Simpson's $\frac{3}{8}$ rule integrates $y = P_3(x)$ over $[x_0, x_3] = [0.0, 1.5]$. (d) Boole's rule integrates $y = P_4(x)$ over $[x_0, x_4] = [0.0, 2.0]$.

Corollary 7.1 (Newton-Cotes Precision). Assume that $f(x)$ is sufficiently differentiable; then $E[f]$ for Newton-Cotes quadrature involves an appropriate higher derivative. The trapezoidal rule has degree of precision $n = 1$. If $f \in C^2[a, b]$, then

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12} f^{(2)}(c). \tag{8}$$

Simpson's rule has degree of precision $n = 3$. If $f \in C^4[a, b]$, then

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90} f^{(4)}(c). \tag{9}$$

Simpson's $\frac{3}{8}$ rule has degree of precision $n = 3$. If $f \in C^4[a, b]$, then

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80} f^{(4)}(c). \tag{10}$$

Boole's rule has degree of precision $n = 5$. If $f \in C^6[a, b]$, then

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) - \frac{8h^7}{945} f^{(6)}(c). \tag{11}$$

Proof of Theorem 7.1. Start with the Lagrange polynomial $P_M(x)$ based on x_0, x_1, $\ldots$, x_M that can be used to approximate $f(x)$:

$$f(x) \approx P_M(x) = \sum_{k=0}^{M} f_k L_{M,k}(x), \tag{12}$$

where $f_k = f(x_k)$ for $k = 0, 1, \ldots, M$. An approximation for the integral is obtained by replacing the integrand $f(x)$ with the polynomial $P_M(x)$. This is the general method for obtaining a Newton-Cotes integration formula:

$$\begin{aligned}\int_{x_0}^{x_M} f(x)\,dx &\approx \int_{x_0}^{x_M} P_M(x)\,dx\\ &= \int_{x_0}^{x_M} \left(\sum_{k=0}^{M} f_k L_{M,k}(x)\right) dx = \sum_{k=0}^{M}\left(\int_{x_0}^{x_M} f_k L_{M,k}(x)\,dx\right)\\ &= \sum_{k=0}^{M}\left(\int_{x_0}^{x_M} L_{M,k}(x)\,dx\right) f_k = \sum_{k=0}^{M} w_k f_k.\end{aligned} \tag{13}$$

The details for the general computations of the coefficients of w_k in (13) are tedious. We shall give a sample proof of Simpson's rule, which is the case $M = 2$. This case involves the approximating polynomial

$$P_2(x) = f_0\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f_1\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}. \tag{14}$$

Since f_0, f_1, and f_2 are constants with respect to integration, the relations in (13) lead to

$$\begin{aligned}\int_{x_0}^{x_2} f(x)\,dx \approx f_0\int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\,dx + f_1\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\,dx\\ + f_2\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}\,dx.\end{aligned} \tag{15}$$

We introduce the change of variable $x = x_0 + ht$ with $dx = h\,dt$ to assist with the evaluation of the integrals in (15). The new limits of integration are from $t = 0$ to $t = 2$. The equal spacing of the nodes $x_k = x_0 + kh$ leads to $x_k - x_j = (k - j)h$ and

$x - x_k = h(t-k)$, which are used to simplify (15) and get

(16)

$$\begin{aligned}
\int_{x_0}^{x_2} f(x)\,dx &\approx f_0 \int_0^2 \frac{h(t-1)h(t-2)}{(-h)(-2h)} h\,dt + f_1 \int_0^2 \frac{h(t-0)h(t-2)}{(h)(-h)} h\,dt \\
&\quad + f_2 \int_0^2 \frac{h(t-0)h(t-1)}{(2h)(h)} h\,dt \\
&= f_0 \frac{h}{2} \int_0^2 (t^2 - 3t + 2)\,dt - f_1 h \int_0^2 (t^2 - 2t)\,dt + f_2 \frac{h}{2} \int_0^2 (t^2 - t)\,dt \\
&= f_0 \frac{h}{2} \left(\frac{t^3}{3} - \frac{3t^2}{2} + 2t \right) \Bigg|_{t=0}^{t=2} - f_1 h \left(\frac{t^3}{3} - t^2 \right) \Bigg|_{t=0}^{t=2} \\
&\quad + f_2 \frac{h}{2} \left(\frac{t^3}{3} - \frac{t^2}{2} \right) \Bigg|_{t=0}^{t=2} \\
&= f_0 \frac{h}{2} \left(\frac{2}{3} \right) - f_1 h \left(\frac{-4}{3} \right) + f_2 \frac{h}{2} \left(\frac{2}{3} \right) \\
&= \frac{h}{3} (f_0 + 4f_1 + f_2),
\end{aligned}$$

and the proof is complete. We postpone a sample proof of Corollary 7.1 until Section 7.2. •

Example 7.1. Consider the function $f(x) = 1 + e^{-x}\sin(4x)$, the equally spaced quadrature nodes $x_0 = 0.0$, $x_1 = 0.5$, $x_2 = 1.0$, $x_3 = 1.5$, and $x_4 = 2.0$, and the corresponding function values $f_0 = 1.00000$, $f_1 = 1.55152$, $f_2 = 0.72159$, $f_3 = 0.93765$, and $f_4 = 1.13390$. Apply the various quadrature formulas (4) through (7).

The step size is $h = 0.5$, and the computations are

$$\begin{aligned}
\int_0^{0.5} f(x)\,dx &\approx \frac{0.5}{2}(1.00000 + 1.55152) = 0.63788 \\
\int_0^{1.0} f(x)\,dx &\approx \frac{0.5}{3}(1.00000 + 4(1.55152) + 0.72159) = 1.32128 \\
\int_0^{1.5} f(x)\,dx &\approx \frac{3(0.5)}{8}(1.00000 + 3(1.55152) + 3(0.72159) + 0.93765) \\
&= 1.64193 \\
\int_0^{2.0} f(x)\,dx &\approx \frac{2(0.5)}{45}(7(1.00000) + 32(1.55152) + 12(0.72159) \\
&\qquad + 32(0.93765) + 7(1.13390)) = 2.29444.
\end{aligned}$$

■

It is important to realize that the quadrature formulas (4) through (7) applied in the illustration above give approximations for definite integrals over different intervals.

The graph of the curve $y = f(x)$ and the areas under the Lagrange polynomials $y = P_1(x)$, $y = P_2(x)$, $y = P_3(x)$, and $y = P_4(x)$ are shown in Figure 7.2(a) through (d), respectively.

In Example 7.1 we applied the quadrature rules with $h = 0.5$. If the endpoints of the interval $[a, b]$ are held fixed, the step size must be adjusted for each rule. The step sizes are $h = b - a$, $h = (b - a)/2$, $h = (b - a)/3$, and $h = (b - a)/4$ for the trapezoidal rule, Simpson's rule, Simpson's $\frac{3}{8}$ rule, and Boole's rule, respectively. The next example illustrates this point.

Example 7.2. Consider the integration of the function $f(x) = 1 + e^{-x}\sin(4x)$ over the fixed interval $[a, b] = [0, 1]$. Apply the various formulas (4) through (7).

For the trapezoidal rule, $h = 1$ and

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{1}{2}(f(0) + f(1))\\ &= \frac{1}{2}(1.00000 + 0.72159) = 0.86079.\end{aligned}$$

For Simpson's rule, $h = 1/2$, and we get

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{1/2}{3}(f(0) + 4f(\tfrac{1}{2}) + f(1))\\ &= \frac{1}{6}(1.00000 + 4(1.55152) + 0.72159) = 1.32128.\end{aligned}$$

For Simpson's $\frac{3}{8}$ rule, $h = 1/3$, and we obtain

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{3(1/3)}{8}(f(0) + 3f(\tfrac{1}{3}) + 3f(\tfrac{2}{3}) + f(1))\\ &= \frac{1}{8}(1.00000 + 3(1.69642) + 3(1.23447) + 0.72159) = 1.31440.\end{aligned}$$

For Boole's rule, $h = 1/4$, and the result is

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{2(1/4)}{45}(7f(0) + 32f(\tfrac{1}{4}) + 12f(\tfrac{1}{2}) + 32f(\tfrac{3}{4}) + 7f(1))\\ &= \frac{1}{90}(7(1.00000) + 32(1.65534) + 12(1.55152)\\ &\quad + 32(1.06666) + 7(0.72159)) = 1.30859.\end{aligned}$$

The true value of the definite integral is

$$\int_0^1 f(x)\,dx = \frac{21e - 4\cos(4) - \sin(4)}{17e} = 1.3082506046426\ldots,$$

and the approximation 1.30859 from Boole's rule is best. The area under each of the Lagrange polynomials $P_1(x)$, $P_2(x)$, $P_3(x)$, and $P_4(x)$ is shown in Figure 7.3(a) through (d), respectively. ■

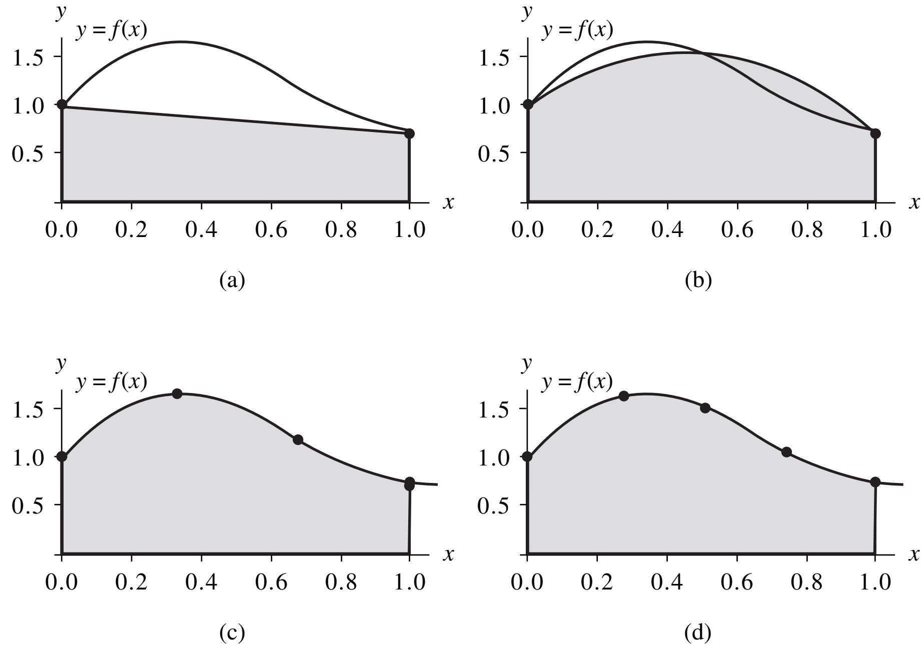


Figure 7.3 (a) The trapezoidal rule used over [0, 1] yields the approximation 0.86079. (b) Simpson's rule used over [0, 1] yields the approximation 1.32128. (c) Simpson's $\frac{3}{8}$ rule used over [0, 1] yields the approximation 1.31440. (d) Boole's rule used over [0, 1] yields the approximation 1.30859.

To make a fair comparison of quadrature methods, we must use the same number of function evaluations in each method. Our final example is concerned with comparing integration over a fixed interval $[a, b]$ using exactly five function evaluations $f_k = f(x_k)$, for $k = 0, 1, \ldots, 4$ for each method. When the trapezoidal rule is applied on the four subintervals $[x_0, x_1]$, $[x_1, x_2]$, $[x_2, x_3]$, and $[x_3, x_4]$, it is called a ***composite trapezoidal rule***:

$$
\begin{aligned}
\int_{x_0}^{x_4} f(x)\,dx &= \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \int_{x_2}^{x_3} f(x)\,dx + \int_{x_3}^{x_4} f(x)\,dx \\
&\approx \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \frac{h}{2}(f_2 + f_3) + \frac{h}{2}(f_3 + f_4) \qquad (17) \\
&= \frac{h}{2}(f_0 + 2f_1 + 2f_2 + 2f_3 + f_4).
\end{aligned}
$$

Simpson's rule can also be used in this manner. When Simpson's rule is applied on the two subintervals $[x_0, x_2]$ and $[x_2, x_4]$, it is called a ***composite Simpson's rule***:

$$\begin{aligned} \int_{x_0}^{x_4} f(x)\,dx &= \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx \\ &\approx \frac{h}{3}(f_0 + 4f_1 + f_2) + \frac{h}{3}(f_2 + 4f_3 + f_4) \\ &= \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4). \end{aligned} \tag{18}$$

The next example compares the values obtained with (17), (18), and (7).

Example 7.3. Consider the integration of the function $f(x) = 1 + e^{-x}\sin(4x)$ over $[a, b] = [0, 1]$. Use exactly five function evaluations and compare the results from the composite trapezoidal rule, composite Simpson rule, and Boole's rule.

The uniform step size is $h = 1/4$. The composite trapezoidal rule (17) produces

$$\begin{aligned} \int_0^1 f(x)\,dx &\approx \frac{1/4}{2}\left(f(0) + 2f(\tfrac{1}{4}) + 2f(\tfrac{1}{2}) + 2f(\tfrac{3}{4}) + f(1)\right) \\ &= \frac{1}{8}(1.00000 + 2(1.65534) + 2(1.55152) + 2(1.06666) + 0.72159) \\ &= 1.28358. \end{aligned}$$

Using the composite Simpson's rule (18), we get

$$\begin{aligned} \int_0^1 f(x)\,dx &\approx \frac{1/4}{3}\left(f(0) + 4f(\tfrac{1}{4}) + 2f(\tfrac{1}{2}) + 4f(\tfrac{3}{4}) + f(1)\right) \\ &= \frac{1}{12}(1.00000 + 4(1.65534) + 2(1.55152) + 4(1.06666) + 0.72159) \\ &= 1.30938. \end{aligned}$$

We have already seen the result of Boole's rule in Example 7.2:

$$\begin{aligned} \int_0^1 f(x)\,dx &\approx \frac{2(1/4)}{45}\left(7f(0) + 32f(\tfrac{1}{4}) + 12f(\tfrac{1}{2}) + 32f(\tfrac{3}{4}) + 7f(1)\right) \\ &= 1.30859. \end{aligned}$$

The true value of the integral is

$$\int_0^1 f(x)\,dx = \frac{21e - 4\cos(4) - \sin(4)}{17e} = 1.3082506046426\ldots,$$

and the approximation 1.30938 from Simpson's rule is much better than the value 1.28358 obtained from the trapezoidal rule. Again, the approximation 1.30859 from Boole's rule is closest. Graphs for the areas under the trapezoids and parabolas are shown in Figure 7.4(a) and (b), respectively. ■

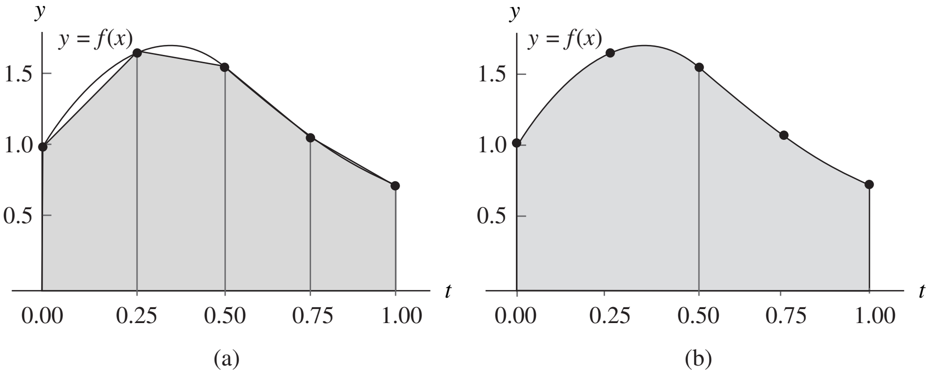


Figure 7.4 (a) The composite trapezoidal rule yields the approximation 1.28358. (b) The composite Simpson rule yields the approximation 1.30938.

Example 7.4. Determine the degree of precision of Simpson's $\frac{3}{8}$ rule.

It will suffice to apply Simpson's $\frac{3}{8}$ rule over the interval [0, 3] with the five test functions $f(x) = 1, x, x^2, x^3$, and x^4. For the first four functions, Simpson's $\frac{3}{8}$ rule is exact.

$$\begin{aligned}
\int_0^3 1\,dx &= 3 = \frac{3}{8}(1 + 3(1) + 3(1) + 1)\\
\int_0^3 x\,dx &= \frac{9}{2} = \frac{3}{8}(0 + 3(1) + 3(2) + 3)\\
\int_0^3 x^2\,dx &= 9 = \frac{3}{8}(0 + 3(1) + 3(4) + 9)\\
\int_0^3 x^3\,dx &= \frac{81}{4} = \frac{3}{8}(0 + 3(1) + 3(8) + 27).
\end{aligned}$$

The function $f(x) = x^4$ is the lowest power of x for which the rule is not exact.

$$\int_0^3 x^4\,dx = \frac{243}{5} \approx \frac{99}{2} = \frac{3}{8}(0 + 3(1) + 3(16) + 81).$$

Therefore, the degree of precision of Simpson's $\frac{3}{8}$ rule is $n = 3$. ■

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