5. Quadrature

The term *quadrature* has its origin in a simple technique for estimating areas: draw the shape on engineering paper and count the squares. For example, the shaded region in Figure 3 consists of 44 fully and partially filled squares. Therefore

$$\int_0^1 f(x)\, dx \leq 0.44,$$

where f is the function whose graph bounds the region.

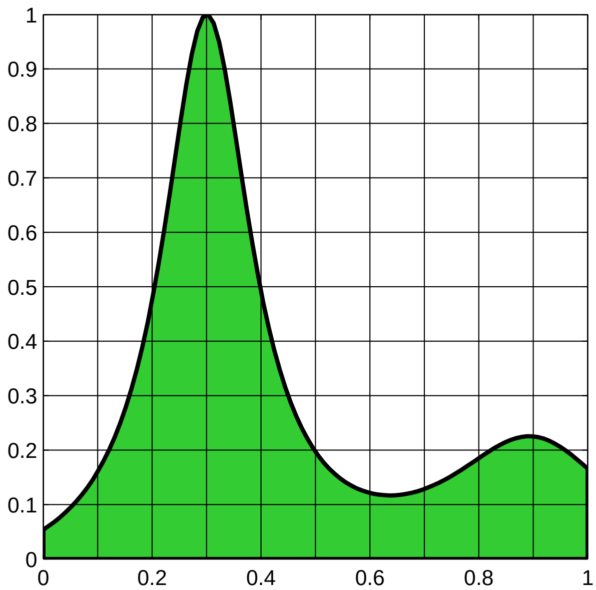

Figure 3. Quadrature in one dimension

As almost every topic in Numerical Analysis, the numerical quadrature is an extensive subject and an area of current research. We will start with quadrature in one dimension where the ideas are easier to bring into focus. Henceforth, our model problem is to approximate the definite integral $\int_a^b f(x)\, dx$ where f is a sufficiently well-behaved function and the limits of integration are finite. Once we understand the principles behind simple one-dimensional quadrature, we will try to extend them to multidimensional integrals and improper integrals[7].

[7]Improper integrals are the ones with infinite limits, integrands having singularities, or both.

5.1. **Quadrature in Calculus.** Figure 4 shows several *composite* quadrature rules that should be familiar from Calculus I.

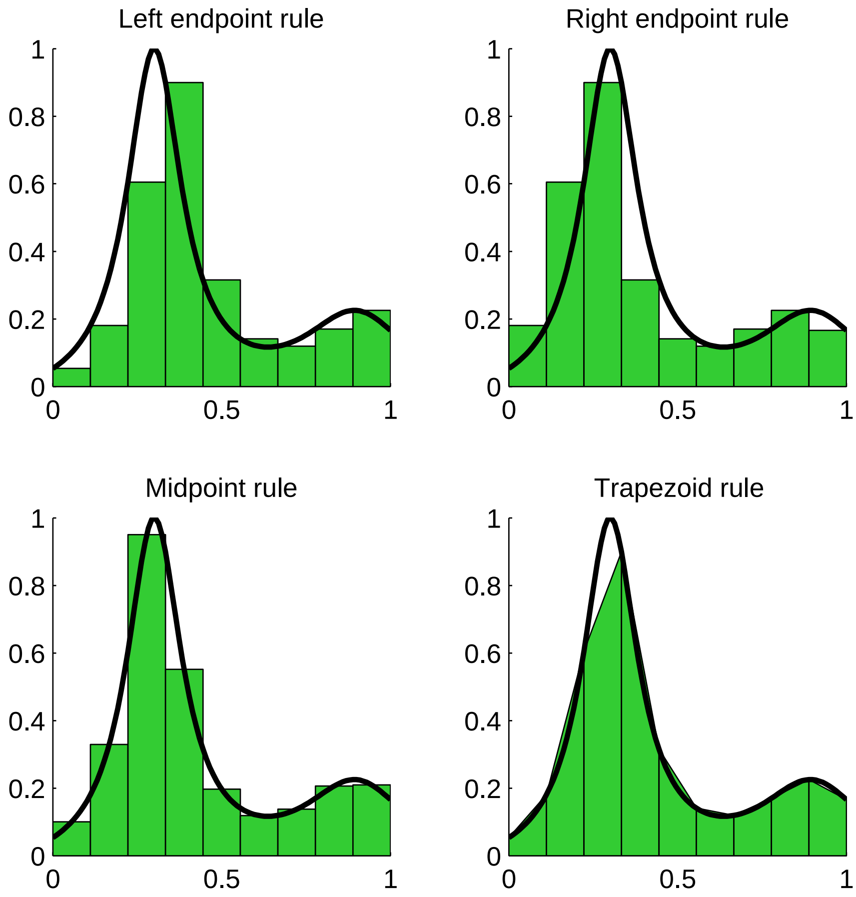

FIGURE 4. Quadrature in Calculus

In the context of quadrature, the word 'composite' simply means that the rule is applied on small subintervals into which the domain is subdivided; the results are then added up. For instance, the actual left endpoint rule stated for the interval $[a, b]$ is, simply:

$$\int_a^b f(x)\,dx \approx f(a)\,(b-a).$$

Suppose now that the interval $[a, b]$ is subdivided into N subintervals. Denote the left endpoint of the n-th subinterval by x_n and its length by Δx_n. The composite left endpoint rule is then:

$$\int_a^b f(x)\,dx \approx \sum_{n=1}^{N} f(x_n)\,\Delta x_n.$$

The analysis of composite rules is straightforward once the rules themselves are understood. With that in mind, we turn our attention to the organizational principle behind quadrature. Can you see what the four methods in Figure 4 have in common?

5.2. **The organizational principle.** There are, literally, infinitely many quadrature rules. However, most of the rules—and certainly the most important ones—are based on the simple principle:

> To approximate $\int_a^b f(x)\,dx$, replace f with an interpolating polynomial[8].

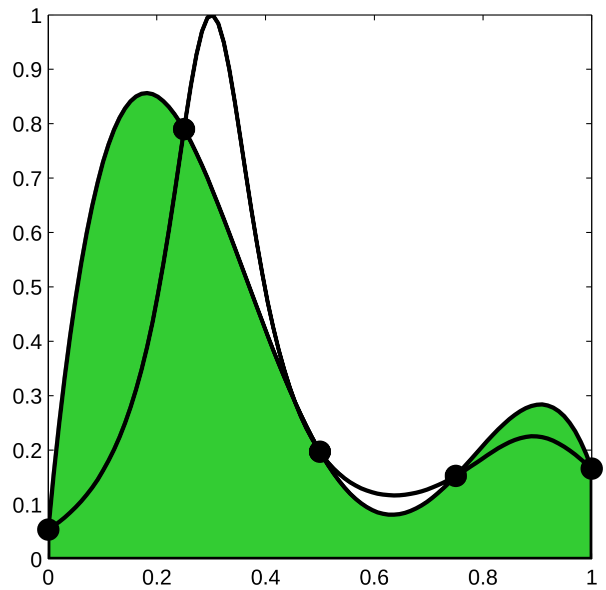

FIGURE 5. Interpolatory quadrature

Since it is often desirable to approximate integrals using only the values of the integrand, we will mostly focus on rules based on Lagrangian interpolation. The latter can be divided into several families differing

[8]Integration of rational functions leads to logarithms which are computationally expensive. Therefore Padé approximation is rarely used in quadrature schemes.

by the choice of nodes. All familiar Calculus rules, as well as the rule illustrated in Figure 5, belong to the class known as Newton-Cotes formulas which we introduce in the next section.

5.3. **Newton-Cotes quadrature rules.** Newton-Cotes rules use equispaced nodes and are divided into two types: open and closed.

Closed rules use the endpoints of the interval as some of the nodes. For example, the closed Newton-Cotes formula with two nodes uses the endpoints of the interval:

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \int_a^b \left(f(a)\,\frac{x-b}{a-b} + f(b)\,\frac{x-a}{b-a} \right) dx \\ &= \frac{1}{2}\,(f(a)+f(b))\,(b-a).\end{aligned} \tag{22}$$

Notice that Equation (22) is just the trapezoid rule.

The next closed formula is obtained by integrating the quadratic interpolant whose nodes are the endpoints and the midpoint. This rule is known as the Simpson's Rule; it is also sometimes called *parabolic rule* for obvious reasons. Let c denote the midpoint of $[a, b]$. Integration of the quadratic interpolant with nodes at a, b, and c leads to:

$$\begin{aligned}\int_a^b f(x)\,dx \approx \int_a^b \Bigg(& f(a)\,\frac{(x-b)(x-c)}{(a-b)(a-c)} + f(b)\,\frac{(x-a)(x-c)}{(b-a)(b-c)} \\ & + f(c)\,\frac{(x-a)(x-b)}{(c-a)(c-b)} \Bigg)\,dx \\ = \; & \frac{1}{6}\,(f(a)+4\,f(c)+f(b))\,(b-a), \quad c = \frac{a+b}{2}.\end{aligned} \tag{23}$$

Here we purposefully omitted the details of algebraic simplification for two reasons. Firstly, they are tedious. Secondly, we would like to encourage the reader to produce Equation (23) independently using a computer algebra system (CAS) such as Maple or Mathematica. The use of CAS will become indispensable when we get to the analysis of errors in quadrature rules.

The closed Newton-Cotes formula based on the cubic interpolant is also attributed to Simpson and is called the Simpson's 3/8 rule. One of the exercises at the end asks you to derive it and explain the name. Higher order Newton-Cotes formulas do not have special names and are, in fact, rarely used in practice.

Open Newton-Cotes formula use only the interior nodes. The simplest example is the midpoint rule:

$$\int_a^b f(x)\,dx \approx \int_a^b f(c)\,dx = f(c)\,(b-a), \quad c = \frac{a+b}{2}.$$

Following that, is the open Newton-Cotes formula with two nodes—it does not have a special name:

$$\int_a^b f(x)\,dx \approx \frac{1}{2}\,(f(x_1)+f(x_2))\,(b-a), \quad x_1 = \frac{2\,a+b}{3}, \quad x_2 = \frac{a+2\,b}{3}.$$

Derivation of other open Newton-Cotes formulas is similar and is relegated to exercises. Here we close with the remark that the reason why open formulas are distinguished from closed formulas is because they apply to integrands with singularities at the endpoints of the interval.

Notice that all Newton-Cotes formulas can be written as linear combinations of function values:

$$\int_a^b f(x)\,dx \approx \sum_{n=1}^{N} w_n\,f(x_n). \tag{24}$$

In Equation (24) x_n's are the (equispaced) nodes (interior for open formulas) and w_n are the *weights* which are also called *Cotes numbers.* As this section shows, the Cotes numbers are obtained simply by integrating the appropriate Lagrangian interpolant.

As we have already suggested, in practice one works with Newton-Cotes rules based on a small number of nodes. The main reason for this is the instability of interpolation. For large numbers of nodes the interpolants oscillate wildly and so do the Cotes numbers. Rules where Cotes numbers are of different signs tend to be numerically unstable and are therefore avoided.

5.4. **Error analysis: take one.** Since quadrature rules are in one way or another based on interpolation, we can easily derive an expression for the error by integrating the remainder. For instance, integration of the linear interpolation formula with the remainder

$$f(x) = f(a)\,\frac{x-b}{a-b} + f(b)\,\frac{x-a}{b-a} + \frac{f''(\xi)}{2}\,(x-a)\,(x-b),$$

leads to the error term for the trapezoid rule (22):

$$\int_a^b f(x)\,dx - \frac{1}{2}\,(f(a)+f(b))\,(b-a) = \int_a^b \frac{f''(\xi(x))}{2}\,(x-a)\,(x-b)\,dx.$$

We wrote $\xi = \xi(x)$ inside the integral to emphasize that ξ cannot be treated as a constant. Nevertheless, since $(x-a)\,(x-b) \leq 0$ for all $x \in [a,b]$, we can use GMVT to pull out the second derivative. This results in

$$
\begin{aligned}
(25)\qquad \int_a^b \frac{f''(\xi(x))}{2}\,(x-a)\,(x-b)\,dx &= \frac{f''(\eta)}{2}\int_a^b (x-a)\,(x-b)\,dx \\
&= -\frac{f''(\eta)}{12}\,(b-a)^3,
\end{aligned}
$$

where η now is a fixed number in $[a, b]$. Equation (25) shows that the trapezoid rule is exact for all polynomials of degree one or less. It further shows that the error of the trapezoid rule depends cubically on the length of the interval. In particular, if the length of the interval is halved, the error decreases by the factor of eight.

Unfortunately, the remainder of the Lagrangian interpolation does not always maintain constant sign on the domain of integration and this limits the use of GMVT. For instance, for the midpoint rule we can certainly write the error as the following integral:

$$\int_a^b f(x)\,dx - f(c)\,(b-a) = \int_a^b f'(\xi(x))\,(x-c)\,dx, \quad c = \frac{a+b}{2}.$$

Yet $(x - c)$ changes sign on $[a, b]$ and GMVT cannot be applied. In order to derive an error term similar to (25), we need a more subtle approach presented in the next section.

5.5. **Take two: Peano Kernel Theorem.** All interpolatory quadrature schemes are, by design, exact for low order polynomials. Let n be the highest degree a polynomial can have so that the quadrature rule produces an exact answer. This nonnegative integer is called the *order of accuracy* of the rule. For instance, both the trapezoid and midpoint rules are of first order. Peano Kernel Theorem expresses the error of interpolatory quadrature as an integral of the form

$$\int_a^b f^{(n+1)}(t)\,K(t)\,dt,$$

where n is the order of accuracy and $K(t)$—the Peano kernel—is independent of f. Unlike the Lagrangian remainder, the Peano kernel tends to maintain constant sign on $[a, b]$. This allows for the use of GMVT leading to error formulas of the type $k\,f^{(n+1)}(\eta)$ with $k = \int_a^b K(t)\,dt$. In order to state Peano's theorem, we need to introduce some language from linear algebra which we proceed to do.

5.5.1. *Linear functionals.* Think of a functional as a procedure that takes a function as an input and produces a real or complex number as an output. For instance, consider the functional L defined by

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

This, clearly, is a familiar object that is of prime interest to us now. However, let us think of the integral differently: not as "the area under the curve" or "the limit of a Riemann sum" but as a "function" operating on functions. The functional L is linear because

$$L(c_1\,f_1 + c_2\,f_2) = c_1\,L(f_1) + c_2\,L(f_2)$$

for any functions f_1, f_2 and constants c_1, c_2. In words, L maps linear combinations of inputs into linear combinations of outputs. Any functional that does not have that property is nonlinear, e.g.:

$$N(f) = \int_a^b f^2(x)\,dx.$$

Linearity is a crucial attribute that is going to be required by our theory. We will therefore only consider linear functionals.

As another example consider the evaluation functional: $f \mapsto f(p)$. This functional simply evaluates a function at some point p and is clearly linear. Any linear combination of linear functionals is itself a linear functional (exercise). In particular, any interpolatory quadrature rule, being a linear combination of evaluation functionals, is a linear functional designed to approximate L.

Let Q be a linear functional that approximates L in some sense. We will call the difference $E = L - Q$ the *error functional* corresponding to Q. For instance, the error functional for the midpoint rule is given explicitly by:

$$E(f) = \int_a^b f(x)\,dx - f\left(\frac{a+b}{2}\right)(b-a). \tag{26}$$

5.5.2. *Peano Kernel Theorem.* Since the midpoint rule is of first order, its error functional E defined by (26) is zero for all linear functions. We will say that E *annihilates* first degree polynomials. Peano observed that something constructive can be said about linear functionals that annihilate polynomials.

Theorem 6 (Peano Kernel Theorem)**.** *Let L be a linear functional acting on smooth functions defined on the interval $[a,b]$. Suppose that L annihilates all polynomials of degree n or less. Then for any $f \in C^\infty([a,b])$:*

$$L(f) = \int_a^b f^{(n+1)}(t)\,K(t)\,dt, \tag{27}$$

where

$$K(t) = \frac{1}{n!} L_x \left((x-t)_+^n \right).$$

The subindex in L_x indicates that the functional is applied in the x-variable; the plus sign in $(x-t)_+^n$ is standard notation for the truncated power function:

$$(x-t)_+^n = \begin{cases} (x-t)^n, & t < x, \\ 0, & \textit{otherwise.} \end{cases}$$

Proof. Let $f \in C^\infty([a,b])$. The Taylor expansion of f to n-th order at $x = a$ can be written as follows:

$$\begin{aligned} f(x) &= f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \dots \\ &+ \frac{f^{(n)}(a)}{n!}(x-a)^n + \int_a^x \frac{(x-t)^n}{n!} f^{(n+1)}(t)\, dt. \end{aligned} \tag{28}$$

Now apply L to Equation (28). Since L is linear and since L annihilates polynomials of degree n or less, the result is:

$$L(f) = L\left(\int_a^x \frac{(x-t)^n}{n!} f^{(n+1)}(t)\, dt \right).$$

To finish the proof, we would like to bring L inside the integral. To do that, introduce the truncated power function and write the integral as follows:

$$\int_a^x \frac{(x-t)^n}{n!} f^{(n+1)}(t)\, dt = \int_a^b \frac{(x-t)_+^n}{n!} f^{(n+1)}(t)\, dt.$$

Now that the limits are constant, L can be brought inside the integral and, since L acts on the variable x, the result is:

$$L(f) = \int_a^b L_x\left(\frac{(x-t)_+^n}{n!} \right) f^{(n+1)}(t)\, dt = \int_a^b K(t)\, f^{(n+1)}(t)\, dt.$$

Which was to be demonstrated. □

Of particular use to us will be the following consequence of Theorem 6.

Corollary 7. *If Peano kernel maintains constant sign on $[a,b]$ then Equation (27) can be rewritten as:*

$$L(f) = f^{(n+1)}(\xi) \int_a^b K(t)\, dt. \tag{29}$$

The proof of Corollary 7 is a straightforward application of GMVT.

5.5.3. *The use of Peano Kernel Theorem.* As an application of Theorem 6, let us find the error of the midpoint rule. Since the rule is of first order, the Peano kernel is obtained by applying the error functional (26) to $(x-t)_+$:

$$K(t) = \int_a^b (x-t)_+\,dx - \left(\frac{a+b}{2} - t\right)_+ (b-a).$$

Since $(x-t)_+ = 0$ as long as $x < t$, we can compute the integral as follows:

$$\int_a^b (x-t)_+\,dx = \int_t^b (x-t)\,dx = \frac{(b-t)^2}{2}.$$

Now, by definition of the truncated power function:

$$\left(\frac{a+b}{2} - t\right)_+ (b-a) = \begin{cases} \left(\frac{a+b}{2} - t\right)(b-a), & a \le t < \frac{a+b}{2}, \\ 0, & \frac{a+b}{2} \le t \le b. \end{cases}$$

Hence

$$\begin{aligned} K(t) &= \frac{(b-t)^2}{2} + \begin{cases} \left(\frac{a+b}{2} - t\right)(b-a), & a \le t < \frac{a+b}{2} \\ 0, & \frac{a+b}{2} \le t \le b \end{cases} \\ &= \begin{cases} \frac{(b-t)^2}{2} + \left(\frac{a+b}{2} - t\right)(b-a), & a \le t < \frac{a+b}{2} \\ \frac{(b-t)^2}{2}, & \frac{a+b}{2} \le t \le b \end{cases} \\ &= \begin{cases} \frac{(a-t)^2}{2}, & a \le t < \frac{a+b}{2}, \\ \frac{(b-t)^2}{2}, & \frac{a+b}{2} \le t \le b. \end{cases} \end{aligned}$$

Evidently, $K(t) \ge 0$ on $[a,b]$. Therefore, by Corollary 7:

$$\begin{aligned} E(f) &= f''(\xi) \int_a^b \left(\begin{cases} \frac{(a-t)^2}{2}, & a \le t < \frac{a+b}{2}, \\ \frac{(b-t)^2}{2}, & \frac{a+b}{2} \le t \le b. \end{cases} \right) dt \\ &= f''(\xi) \left(\int_a^{\frac{a+b}{2}} \frac{(a-t)^2}{2}\,dt + \int_{\frac{a+b}{2}}^b \frac{(b-t)^2}{2}\,dt \right) \\ &= \frac{f''(\xi)}{24}(b-a)^3. \end{aligned}$$

Curiously, the midpoint rule, which uses a single node, is twice as accurate[9] as the trapezoid rule which uses two nodes.

[9]We do not mean to say that in a given situation the error of the midpoint rule will necessarily be half that of the trapezoid rule. The second derivative in the two error terms is evaluated at different ξ. So, it may very well happen that in a particular situation the trapezoid rule outperforms midpoint rule. However, on average, one can expect the midpoint rule to be somewhat more accurate.

5.6. **Error of composite rules.** We will illustrate the analysis of composite quadrature using the trapezoid rule; other composite rules are analyzed in the same manner. Recall that 'composite' means that we break up the interval $[a, b]$ into N subintervals, apply the rule to each subinterval, and add up the results. For simplicity, let us assume that the subdivision is even, so all subintervals have length:

$$h = \frac{b-a}{N}.$$

Let x_n, $n = 0, \ldots, N$ denote equispaced subdivision points with $x_0 = a$ and $x_N = b$. The formula for the composite trapezoid rule has very simple form

$$\frac{f(x_0) + f(x_N)}{2}\, h + h \sum_{n=1}^{N-1} f(x_n) \tag{30}$$

and is implemented in MATLAB as `trapz`.

The error of the composite trapezoid rule is the sum:

$$\sum_{n=1}^{N} \left(-\frac{f''(\eta_n)}{12}\, h^3 \right) = -\frac{h^3}{12} \sum_{n=1}^{N} f''(\eta_n), \quad x_{n-1} \le \eta_n \le x_n. \tag{31}$$

If the second derivative is continuous, which is our tacit assumption, then by IVT:

$$\sum_{n=1}^{N} f''(\eta_n) = N \times \frac{1}{N} \sum_{n=1}^{N} f''(\eta_n) = N\, f''(\xi), \quad a \le \xi \le b.$$

Furthermore, $h\, N = b - a$. Using that, Equation (31) can be simplified to:

$$-\frac{f''(\xi)}{12}\, h^2\, (b-a). \tag{32}$$

To confirm Equation (32), let us apply it to $\int_0^1 x^2\, dx$. Since the length of the interval is one and the second derivative of x^2 is constant, the absolute error is simply:

$$E = \frac{h^2}{6}.$$

Applying the logarithms, we get

$$\log(E) = 2\, \log(h) + \log\left(\frac{1}{6}\right).$$

This means that the log-log plot of the error should produce a straight line with slope two and intercept $\log(1/6)$. This is indeed the case as shown in Figure 6.

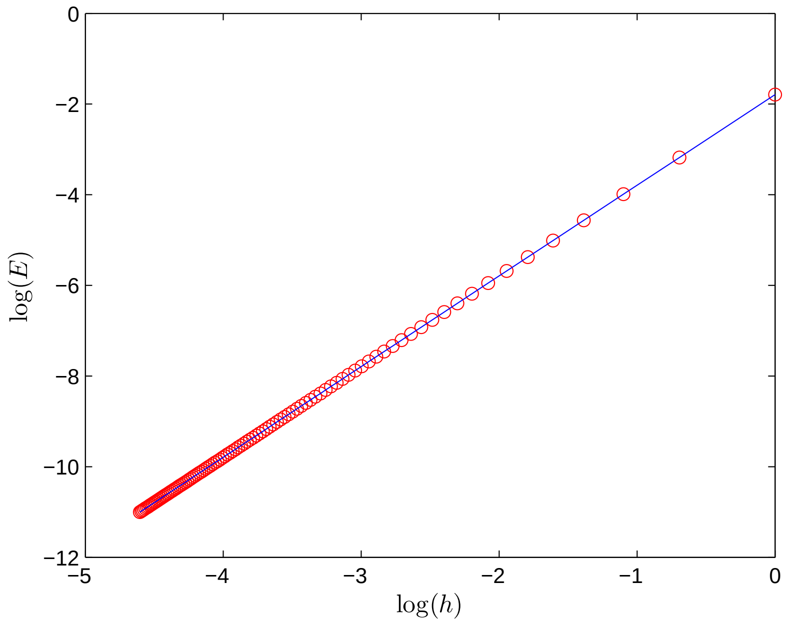

FIGURE 6. The log-log plot of the error of the trapezoid rule applied to $\int_0^1 x^2\,dx$. Plotted in red circles is the data computed using MATLAB's `trapz` command. The best linear fit (blue line) has slope 2 and intercept log(1/6). The fit is perfect because the second derivative of x^2 is constant.

Figure 6 was produced with the following code:

```
f = @(x) x.^2;
I = quad(f,0,1);
h = 1./(1:100);
E = zeros(size(h));
for n=1:length(R)
    x = linspace(0,1,n+1);
    y = f(x);
    Q = trapz(y)*h(n);
    E(n) = abs(I-Q);
end
u = log(h);
v = log(E);
p = polyfit(u,v,1);
plot(u,v,'ro')
```

```
hold on
plot(u,polyval(p,u))
xlabel('$\log(h)$','Interpreter','latex','FontSize',12)
ylabel('$\log(E)$','Interpreter','latex','FontSize',12)
```

For more complicated functions, the fit cannot be perfect, yet it still suggests quadratic dependence in most cases.

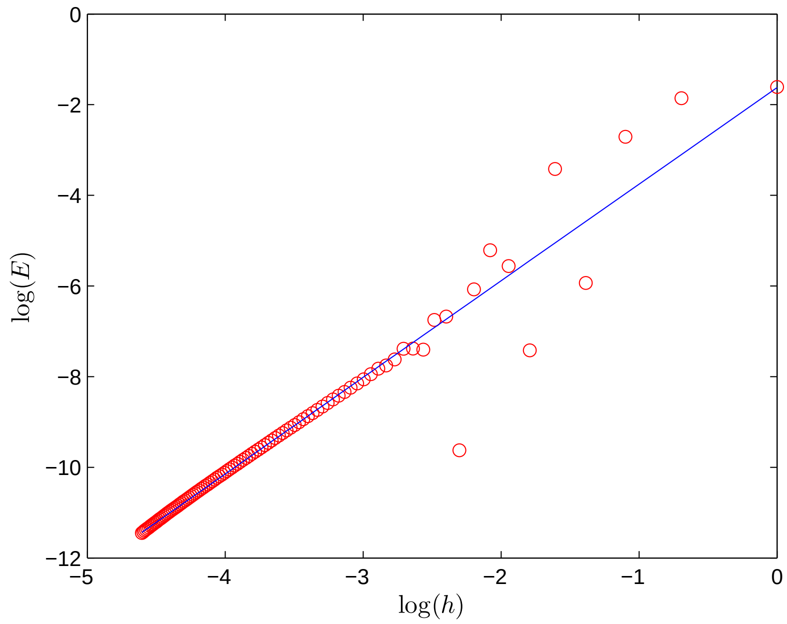

FIGURE 7. The log-log plot of the error of the trapezoid rule applied to $\int_0^1 f(x)\,dx$ where f is the function shown in Figure 3 (MATLAB's `humps` scaled by its maximum). Plotted in red circles is the error of `trapz`; the best linear fit (blue line) now has slope 2.1312 due to noise in the data. The fit still strongly suggests that the error depends quadratically on h.

EXERCISES

(1) Derive the formula for the closed Newton-Cotes rule with four nodes and explain why it is called the Simpson's 3/8 rule. Use CAS if you can.

(2) Use Peano Kernel Theorem to find the error term for the Simpson's Rule. Be sure to provide a clean derivation of the Peano kernel (it will be easier if you use CAS).

(3) Consider the following quadrature rule:
$$\int_{-1}^{+1} f(x)\,dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right).$$
Find the order of accuracy and the error term.

(4) Let
$$D(f) = \frac{f(b) - f(a)}{b - a}$$
be an approximation to $f'(b)$. Find the error of this approximation.

(5) Repeat the previous exercise but regard D as the approximation to $f'(c)$ where $c = \frac{a+b}{2}$.

(6) Let $f \in C^2([a, b])$. Use interpolation to construct a rule for finding the second derivative $f''(b)$ from the function values at five equispaced nodes (CAS is recommended). What is the order of accuracy of the rule? What is the error term?

(7) Derive the error term for composite Simpson's rule. Illustrate it with figures similar to 6 and 7

(8) Confirm numerically that Equation (32) applies to
$$\int_0^{2\pi} \frac{dx}{2 + |\sin(x)|}$$
even though the integrand is not differentiable. How would you explain that?

(9) Perform several numerical experiments where you compare the accuracy of the composite trapezoid and composite midpoint rules. Is it fair to say that the midpoint rule tends to be twice as accurate as trapezoid?

(10) Investigate (numerically) the validity of Equation (32) for the following integral:
$$\int_0^{2\pi} \frac{dx}{2 + \sin(x)}.$$
How fast does the error of the composite trapezoid rule seems to decrease for smooth periodic functions?