A version of Simpson’s rule for multiple integrals

Alan Horwitz
Penn State University, 25 Yearsley Mill Rd., Media, PA 19063, USA
Received 16 August 1999; received in revised form 12 January 2000

Abstract

Let $M(f)$ denote the midpoint rule and $T(f)$ the trapezoidal rule for estimating $\int_a^b f(x) \, dx$. Then Simpson’s rule $S(f) = \lambda M(f) + (1 - \lambda) T(f)$, where $\lambda = \frac{2}{3}$. We generalize Simpson’s rule to multiple integrals as follows. Let $D_n$ be some polygonal region in $\mathbb{R}^n$, let $P_0, \ldots, P_m$ denote the vertices of $D_n$, and let $P_{m+1}$ equal the center of mass of $D_n$. Define the linear functionals $M(f) = \text{Vol}(D_n) f(P_{m+1})$, which generalizes the midpoint rule, and $T(f) = \text{Vol}(D_n) \left( \frac{1}{(m+1)} \sum_{j=0}^{m} f(P_j) \right)$, which generalizes the trapezoidal rule. Finally, our generalization of Simpson’s rule is given by the cubature rule (CR) $L(f) = \lambda M(f) + (1 - \lambda) T(f)$, for fixed $\lambda$, $0 \leq \lambda \leq 1$. We choose $\lambda$, depending on $D_n$, so that $L(f)$ is exact for polynomials of as large a degree as possible. In particular, we derive CRs for the $n$ simplex and unit $n$ cube. We also use points $Q_j \in \partial(D_n)$, other than the vertices $P_j$, to generate $T(f)$. This sometimes leads to better CRs for certain regions — in particular, for quadrilaterals in the plane. We use Grobner bases to solve the system of equations which yield the coordinates of the $Q_j$’s. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Cubature rule; Simpson’s rule; Polygonal region; Grobner basis, exact

1. Introduction

Let $M(f)$ denote the midpoint rule and $T(f)$ the trapezoidal rule for estimating $\int_a^b f(x) \, dx$. Then $M(f)$ and $T(f)$ are each exact for $f(x) = 1$ and $x$. A more accurate rule can be obtained by taking $S(f) = \lambda M(f) + (1 - \lambda) T(f)$, where $\lambda = \frac{2}{3}$. Of course, this rule is known as Simpson’s rule, and is exact for all polynomials of degree $\leq 3$. The purpose of this paper is to use natural generalizations of the midpoint and trapezoidal rules to extend Simpson’s rule to multiple integrals over certain polygonal regions $D_n$ in $\mathbb{R}^n$. First, consider the case $n = 2$. So suppose that $D$ is a polygonal region in $\mathbb{R}^2$. The midpoint rule in one dimension is $M(f) = (b - a) f((a + b)/2)$. A natural extension of this rule is

$$M(f) = A(D) f(P),$$

where $A(D)$ is the area of $D$, and $P$ the centroid of $D$.

E-mail address: alh4@psu.edu (A. Horwitz).
The trapezoidal rule in one dimension is \( T(f) = (b - a)((f(a) + f(b))/2) \). A natural extension of this rule is

\[
T(f) = A(D) \frac{1}{m} \sum_{k=0}^{m} f(P_k),
\]

where the \( P_k \) are the vertices of \( D_n \).

In general, let \( D_n \) be some polygonal region in \( \mathbb{R}^n \), let \( P_0, \ldots, P_m \) denote the vertices of \( D_n \), and let \( P_{m+1} \) be the center of mass of \( D_n \). Define the linear functionals

\[
M(f) = \text{Vol}(D_n) f(P_{m+1}), \quad T(f) = \text{Vol}(D_n) \left( \sum_{j=0}^{m} f(P_j) \right),
\]

and for fixed \( \lambda, 0 \leq \lambda \leq 1 \),

\[
L_\lambda = \lambda M(f) + (1 - \lambda) T(f).
\]

The idea is to choose \( \lambda \) so that \( L_\lambda \) is a good cubature rule (CR). Our objective here is not to provide optimal cubature rules, but to generalize the ideas from Simpson’s rule in one variable to several variables. In some cases we have reproduced known CRs using a different approach.\(^1\) In other cases our CRs appear to be new. In addition, our approach suggest a general method for deriving CRs for polygonal domains.

For the \( n \) cube \([0,1] \times \cdots \times [0,1] \), \( \lambda = 2/3 \), and the CR \( L(f) \) is exact for all polynomials of degree \( \leq 3 \) (see CR3). This, of course, matches the degree of exactness of Simpson’s rule in one variable. For the \( n \) simplex, \( \lambda = (n + 1)/(n + 2) \), and the CR \( L(f) \) is exact for all polynomials of degree \( \leq 2 \) (see CR1).

For regular polygons in the plane with \( m \) sides, our approach fails for \( m > 4 \). For example, if \( D \) is a regular hexagon, then no choice of \( \lambda \) makes \( L_\lambda \) exact for all polynomials of degree \( \leq 2 \). Even for \( m = 4 \), if the polygon is not regular, then our approach fails as well. For example, let \( D \) be the trapezoid with vertices \( \{(0,0), (1,0), (0,1), (1,2)\} \). Again, no choice of \( \lambda \) makes \( L_\lambda \) exact for all polynomials of degree \( \leq 2 \). One can do better, however, by using points \( Q_j \in \partial(D_n) \), other than the vertices of \( D_n \), to generate \( T(f) \). In some cases this leads to better formulas. For example, for the trapezoid \( D \), this leads to a formula which is exact for polynomials of degree \( \leq 2 \) (see CR5).

Choosing points different from the vertices leads to a system of polynomial equations. We use Grobner basis methods (see [2]), along with Maple, to solve such systems when possible. For the \( n \) simplex \( T_n \), we try using the center of mass of the faces of \( T_n \) to generate \( T(f) \) (see CR2).

A similar idea works for the \( n \) cube.

Instead of using the weighted combination, \( \lambda M(f) + (1 - \lambda) T(f) \), another way to derive Simpson’s rule in one variable is to integrate the quadratic interpolant to \( f \) at \( a, (a + b)/2, \) and \( b \). For the \( n \) simplex \( T_n \), our generalization \( L_\lambda \) can be obtained in a similar fashion by integrating \( p(\hat{x}) \) over \( T_n \), where \( p(\hat{x}) \) is the unique interpolant to \( f(\hat{x}) \) at the vertices and center of mass of \( T_n \). For any region \( D_n \), \( M(f) = \int_{D_n} T(\hat{x}) \, dV \), where \( T(\hat{x}) \) is the tangent hyperplane to \( f(\hat{x}) \) at the center of mass of \( D_n \). For the specific region \( T_n \), \( T(f) = \int_{T_n} L(\hat{x}) \, dV \), where \( L(\hat{x}) \) is the bilinear interpolant to \( f(\hat{x}) \) at the vertices of \( T_n \). This, of course, is the generalization from one variable, where the trapezoidal rule can be obtained by integrating the linear interpolant to \( f \) at the endpoints. For regions \( D_n \) in general, however, \( L_\lambda \) and \( T \) do not always arise in this fashion. Indeed, the number of basis functions does not always match the number of nodes, and the interpolant may not be unique. This is what occurs for the \( n \) cube.

\(^1\) See [1,4] for a thorough treatment of CRs.
We also give an analogous formula, using four knots, for the unit disc (see CR6).
Finally, we note that for most of our CRs, all of the weights are positive, all of the knots lie
inside the region $D_n$, and all but one of the knots lies on the boundary of the region.  

2. $n$ Simplex

Let $P_0, \ldots, P_n$ denote the $n + 1$ vertices of the $n$ simplex $T_n \subset \mathbb{R}^n$. Hence, $P_k = (0, 0, \ldots, 1, 0, 0)$ for $k \geq 1$, and $P_0 = (0, 0, \ldots, 0)$, $\hat{x} = (x_1, \ldots, x_n)$, $dV$ is the standard Lebesgue measure on $T_n$. We list the following useful facts, where $I(f) = \int_{T_n} f(\hat{x}) dV$:

- $\text{Vol}(T_n) = \frac{1}{n!}$, $P_{n+1}$ = center of mass of $T_n = (1/(n + 1), \ldots, 1/(n + 1))$,
- $I(x_k) = 1/(n + 1)!$, $I(x_k^2) = 2/(n + 2)!$, $k = 1, \ldots, n$, $I(x_jx_k) = 1/(n + 2)!$, $j \neq k$. Define the linear functionals
  
  $M(f) = \text{Vol}(T_n) f(P_{n+1}) = \frac{1}{n!} f(1/(n + 1), \ldots, 1/(n + 1))$, 
  
  $T(f) = \text{Vol}(T_n) \left( \frac{1}{n + 1} \sum_{j=0}^{n} f(P_j) \right) = \frac{1}{(n + 1)!} \sum_{j=0}^{n} f(P_j)$

and for fixed $\lambda$, $0 \leq \lambda \leq 1$,

$L_\lambda = \lambda M(f) + (1 - \lambda) T(f)$.

First, $I(x_k) = M(x_k) = T(x_k) = 1/(n + 1)!$ for any $\lambda$. For $j \neq k$, $I(x_jx_k) = 1/(n + 2)!$, $M(x_jx_k) = 1/(n + 1)(n + 1)!$, $T(x_jx_k) = 0$. Hence $L_\lambda(x_jx_k) = I(x_jx_k) \Rightarrow \lambda(1/(n + 1)(n + 1)!)=1/(n + 2)! \Rightarrow \lambda = (n + 1)/(n + 2)$.

Letting $L = L_\lambda$ with this $\lambda$ yields

$L(x_k^2) = \frac{n + 1}{n + 2} \frac{1}{n!} \frac{1}{(n + 1)^2} + \frac{1}{n + 2} \frac{1}{(n + 1)!} = \frac{2}{(n + 2)!} = I(x_k^2)$.

We summarize

CR1.

$L(f) = \frac{n + 1}{(n + 2)n!} f(P_{n+1}) + \frac{1}{(n + 2)!} \sum_{j=0}^{n} f(P_j)$

is exact for all polynomials of degree $\leq 2$. $L$ is not exact for all polynomials of degree $\leq 3$.

For example, if $f(\hat{x}) = x_jx_kx_l$, $j \neq k$, $k \neq l$, $j \neq l$, then $I(f) = 1/(n + 3)!$, while $L(f) = 1/(n + 1)(n + 2)! \neq I(f)$.

2.1. Connection with interpolation

Another way to derive Simpson’s rule in one variable is by using quadratic interpolation at
$a, (a + b)/2, b$. The cubature rule $L(f)$ above can also be obtained by integrating a certain second

---

2 For another generalization of Simpson’s rule, see [3].
degree interpolant to \( f \) over \( T_n \). Let

\[
p(x_1, \ldots, x_n) = A_{n+1}x_1x_2 + \sum_{k=1}^{n} A_kx_k + A_0.
\]

We wish to choose the \( A_k \) so that \( p(P_k) = f(P_k), \) \( k = 0, \ldots, n + 1 \). It follows easily that \( A_0 = f(P_0), \) \( A_k = f(P_k), \) \( k = 1, \ldots, n \), and \( A_{n+1} = f(P_{n+1}) - (n + 1) \sum_{k=0}^{n} f(P_k) \). Hence

\[
\int_{T_n} p(\hat{x}) \, dV = A_{n+2} \frac{1}{(n+2)!} + \frac{1}{(n+1)!} \sum_{k=1}^{n} A_k + \frac{1}{n!} A_0
\]

\[
= \frac{1}{(n+2)!} \left( (n+1)^2 f(P_{n+1}) - (n + 1) \sum_{k=0}^{n} f(P_k) \right)
\]

\[
+ \frac{1}{(n+1)!} \left( \sum_{k=1}^{n} f(P_k) - nf(P_0) \right) + \frac{1}{n!} f(P_0)
\]

\[
= \frac{(n+1)^2}{(n+2)!} f(P_{n+1}) + \frac{1}{(n+2)!} \sum_{k=0}^{n} f(P_k) = L(f).
\]

**Remark 1.** Our quadratic interpolant only uses one second degree basis function. Using the basis functions \( \{1, x_1, \ldots, x_n, x_1x_2\} \), one obtains exactness for \((n^2 + n - 2)/2\) additional quadratic terms.

**Remark 2.** One can also obtain the rule \( T(f) \) using interpolation. \( T(f) = \int_{T_n} q(\hat{x}) \, dV \), where \( q(x_1, \ldots, x_n) = \sum_{k=1}^{n} B_k x_k + B_0 \), the \( B_k \) chosen so that \( q(P_k) = f(P_k), \) \( k = 0, \ldots, n \).

2.2. Other boundary points

It is interesting to examine what happens if we use other points on \( \hat{c}(S_n) \) to generate \( T(f) \). We first examine \( n = 2 \) in some detail, and then generalize.

2.2.1. \( n = 2 \)

Let \( T_2 \) the triangle in \( \mathbb{R}^2 \) with vertices \( \{(0,0),(1,0),(0,1)\} \). Use the points \((a,0),(0,b),(c,1-c), \) \( 0 \leq a \leq 1, \) \( 0 \leq b \leq 1, \) \( 0 \leq c \leq 1 \) from each side of \( T_2 \) to define

\[
T(f) = \text{Area}(T_2) \frac{1}{2} (f(a,0) + f(0,b) + f(c,1-c)) = \frac{1}{2} (f(a,0) + f(0,b) + f(c,1-c)),
\]

\[
M(f) = \frac{1}{2} f(\frac{1}{3}, \frac{1}{3}) \text{ and } L_1 = \lambda M(f) + (1 - \lambda)T(f).
\]

Setting \( L_1(f) = I(f) \) yields the system of equations \( \frac{1}{6} \lambda + \frac{1}{6} (1 - \lambda)(a+c) = \frac{1}{6} \), \( \frac{1}{6} \lambda + \frac{1}{6} (1 - \lambda)(b + 1 - c) = \frac{1}{6} \), \( \frac{1}{6} \lambda + \frac{1}{6} (1 - \lambda)(a^2 + c^2) = \frac{1}{12} \), \( \frac{1}{12} \lambda + \frac{1}{12} (1 - \lambda)(b^2 + (1 - c)^2) = \frac{1}{12} \). We found the following Grobner basis using Maple:

\[
\{-12c^2 + 12\lambda c^2 + 4\lambda - 3 + 12c - 12\lambda c, -1 + a + c, b - c\}.
\]

Setting each polynomial from the Grobner basis to 0 yields precisely the same solutions as the original system. Hence \( b = c, \) \( a = 1 - c, \) and \( \lambda = \frac{12c^2 + 3 - 12c}{12c^2 + 4 - 12c}, \) \( 1 - \lambda = \frac{1}{4(3c^2 + 1 - 3c)} \). Using this
expression for $\lambda$ in terms of $c$, we want to choose $c$ so that $L_\lambda$ is exact for quadratics. With $L_\lambda(f) = \lambda \frac{1}{2} f(1/3,1/3) + (1 - \lambda) \frac{1}{6} (f(1 - c, 0) + f(0,c) + f(c,1 - c))$, we have $L_\lambda(x^2) = L_\lambda(y^2) = \frac{1}{12}$ and $L_\lambda(xy) = \frac{1}{24}$. Hence $L_\lambda(f) = \int_{T_3} f(x,y) dA$ for any quadratic $f(x,y)$ and for any value of $c$. Now setting $L_\lambda(x^3) = I(x^3)$ and $L_\lambda(y^3) = I(y^3)$ yields $c = \frac{1}{2} \pm \frac{1}{\sqrt{353}} \approx 0.42167$. However, using either value of $c$, $L_\lambda(x^2y) \neq I(x^2y)$. Thus $L_\lambda$ is not exact for all cubics.

Hence we have the family of CRs

$$L(f) = \hat{\lambda} \left( \frac{1}{2} \right) f(1/3,1/3) + (1 - \hat{\lambda}) \left( \frac{1}{6} \right) (f(1 - c, 0) + f(0,c) + f(c,1 - c))$$

where $0 \leq c \leq 1$ and $\hat{\lambda} = \frac{12c^3 + 3 - 12c}{12c^3 + 4 - 12c}$.

Remark 3. The CR above, with $c = \frac{1}{2}$, is given in the well known book of Stroud (see [4]), as one of a group of formulas for the triangle $T_2$.

2.2.2. General $n$

For $T_2$ above we used the midpoints of the edges for $T(f)$, so it is natural to try using the center of mass of the faces of $T_n$, given by $Q_k = (1/n,1/n,\ldots,0,\ldots,1/n)$ (all coordinates $1/n$ except the $k$th coordinate $= 0$), $k = 1,\ldots,n$. This yields $T(f) = (1/(n + 1)!) \sum_{k=1}^{n+1} f(Q_k)$. As earlier, $M(f) = (1/n!) f(1/(n+1),\ldots,1/(n+1))$ and $L_\lambda = \lambda M(f) + (1 - \lambda) T(f)$. A simple computation shows that $L_\lambda$ is exact for $x_i$ for any $\lambda$, and is exact for $x_j x_k$, $j \neq k$, if $(1/(n+1))\lambda + ((n - 1)/n^2)(1 - \lambda) = 1/(n + 2)$. This gives $\lambda = -(n - 2)(n+1)/(n + 2)$. With this $\lambda$, we have CR2.

$$L(f) = -(n-2) \frac{n+1}{n+2} \frac{n+1}{n+2} f(1/(n+1),\ldots,1/(n+1)) + \frac{n^2}{(n+2)!} \sum_{k=1}^{n+1} f(Q_k)$$

is exact for all polynomials of degree $\leq 2$. Note that one of the weights is $< 0$ if $n \geq 3$.

Remark 4. It would be nice to choose points on the faces which yield $\hat{\lambda} \geq 0$, and in particular $\hat{\lambda} = 0$. We tried this for $n = 3$, using points on each face of the simplex $T_3$. Let $Q_1 = (a_1,a_2,0)$, $Q_2 = (a_3,0,a_4)$, $Q_3 = (0,a_5,a_6)$, $Q_4 = (a_7,a_8,1 - a_7 - a_8)$, with $a_j \geq 0 \forall j$, $a_j + a_{j+1} \leq 1$, $j = 1,3,5,7$, $T(f) = \text{area}(T_3) \frac{1}{4} \sum_{j=1}^{4} f(Q_j)$, $M(f) = \frac{1}{6} f(\frac{1}{4},\frac{1}{4},\frac{1}{4})$, and $L_\lambda = \lambda M(f) + (1 - \lambda) T(f)$.

The equations giving exactness for $x,y,z,x^2,y^2,z^2,xy,xz,yz$, after some simplification, have the two solutions:

- $a_1 = a_2 = a_4 = a_6 = a_7 = a_8 = 0$, $a_3 = a_4 = 1$, $\lambda = \frac{4}{3}$, which uses the vertices of $T_3$ for $Q_j$, and
- $a_j = \frac{1}{3}$ for all $j$, $\lambda = -\frac{4}{3}$, which uses the center of mass of each face of $T_3$ for $Q_j$.

There may be other solutions as well. In particular, we applied Grobner basis methods to the above equations, along with $\hat{\lambda} = 0$. We were then able to show that there is no solution, and hence
one cannot make $\lambda = 0$. We were not able to find any positive values for $\lambda$, other than $\lambda = \frac{4}{3}$, though it is possible that such values exist.

3. Unit $n$ cube

Let $C_n = [0,1]^n \subset \mathbb{R}^n$, and let $P_0,\ldots,P_{m-1}$ denote the $m$ vertices of $C_n$, $m = 2^n$. Assume that $P_0 = (0,\ldots,0)$ and $P_{m-1} = (1,\ldots,1)$. The other vertices have at least one coordinate which equals 0, and at least one coordinate which equals 1. Let $\hat{x} = (x_1,\ldots,x_n), dV$ the standard Lebesgue measure on $C_n$. We list the following useful facts:

$$\text{vol}(C_n) = 1, \text{ center of mass } = P_m = (\frac{1}{2},\ldots,\frac{1}{2}).$$

For any nonnegative $r_1,\ldots,r_n$,

$$\int_{C_n} x_1^{r_1} x_2^{r_2} \cdots x_n^{r_n} \, dV = \frac{1}{r_1 + 1} \frac{1}{r_2 + 1} \cdots \frac{1}{r_j + 1}.$$

Define the linear functionals

$$M(f) = \text{Vol}(C_n) f(P_m) = f(\frac{1}{2},\ldots,\frac{1}{2}),$$

$$T(f) = \text{Vol}(C_n) \left( \frac{1}{m} \sum_{j=0}^{m-1} f(P_j) \right) = \frac{1}{m} \sum_{j=0}^{m-1} f(P_j),$$

$$I(f) = \int_{C_n} f(\hat{x}) \, dV$$

and for fixed $\lambda$, $0 \leq \lambda \leq 1$, $L_{\lambda} = \lambda M(f) + (1 - \lambda)T(f)$. First, $M(x_k) = T(x_k) = \frac{1}{2}$, which implies that $L_{\lambda}(x_k) = I(x_k)$ for any $\lambda$. For $j \neq k$, $M(x_j x_k) = \frac{1}{4}$, and since there are $2^{n-2}$ ways to get a 1 in both the $j$th and $k$th coordinates of a vertex of $D$, $T(x_j x_k) = (1/m)2^{n-2} = \frac{1}{4}$. Again, $L_{\lambda}(x_j x_k) = I(x_j x_k)$ for any $\lambda$. $M(x_k^2) = \frac{1}{4}$ and $T(x_k^2) = \frac{1}{2}$. Hence $L_{\lambda}(x_k^2) = I(x_k^2) = \frac{1}{3} \Rightarrow \lambda = \frac{2}{3}$. Now consider third degree terms. First, for distinct $i,j,k$, $T(x_i x_j x_k) = M(x_i x_j x_k) = I(x_i x_j x_k) = \frac{1}{8} \Rightarrow L_{2/3}(x_i x_j x_k) = I(x_i x_j x_k)$ for any $\lambda$. Second, for $j \neq k$, $T(x_j^2 x_k) = \frac{1}{8}$, $M(x_j^2 x_k) = \frac{1}{8}$, and $I(x_j^2 x_k) = \frac{1}{8}$, and hence $L_{2/3}(x_j^2 x_k) = I(x_j^2 x_k)$. Finally, $T(x_k^3) = \frac{1}{2}$, $M(x_k^3) = \frac{1}{8}$, and $I(x_k^3) = \frac{1}{4}$, which implies that $L_{2/3}(x_k^3) = I(x_k^3)$. We summarize

CR3. $L(f) = \frac{2}{3} f(\frac{1}{2},\ldots,\frac{1}{2}) + \frac{1}{3} (1/2^n) \sum_{j=0}^{2^n-1} f(P_j)$ is exact for all polynomials of degree $\leq 3$.

Remark 5. If $f(x) = x_k^4$, then $T(f) = \frac{1}{2}$, $M(f) = \frac{1}{16}$, and $I(f) = \frac{1}{8} \Rightarrow \frac{2}{3} M(f) + \frac{1}{3} T(f) = I(f)$. Hence $L$ is not exact in general for polynomials of degree $\leq 4$.

Remark 6. The weights of CR3 are of a special form. Using the nodes $P_0,\ldots,P_m$ above, one might attempt to choose general weights $w_0,\ldots,w_m$ such that the CR $\sum_{j=0}^{m} w_j f(P_j)$ is exact for polynomials of degree $\leq N$, $N$ as large as possible. This involves the solution of a system of linear equations. For the plane ($m = 4$), if $N = 3$, there is a unique solution, which of course gives the weights of CR3 above. If $N = 4$, the linear system is inconsistent. Hence the more general weights do not increase the degree of exactness.
3.1. Other points on boundary of \( n \) cube

3.1.1. \( n = 2 \)

Let \( D \) be the unit square. The formulas above use the vertices of \( D \) to generate \( T(f) \). Here we use the points \((a,0),(0,b),(c,1),(1,d)\) on \( \partial D \), \( a,b,c,d \in [0,1] \), to define \( T(f) = \frac{1}{4}(f(a,0) + f(0,b) + f(c,1) + f(1,d)) \). As earlier, \( M(f) = f(\frac{1}{2}, \frac{1}{2}) \) and \( L_2 = \lambda M(f) + (1 - \lambda)T(f) \). Setting \( L_2(f) = I(f) \) for the nine monomials of degree \( \leq 3 \), where \( I(f) = \int_0^1 \int_0^1 f(x,y) \, dy \, dx \), yields a system of nine polynomial equations in nine unknowns. Maple gives the Grobner basis

\[
\{3\lambda + 6d - 2 - 6\lambda d - 6d^2 + 6\lambda d^2, a - d, -1 + b + d, -1 + c + d\}.
\]

Hence \( a = d, \ b = 1 - d, \ c = 1 - d, \) and \( \lambda = (6d^2 - 6d + 2)/(6d^2 - 6d + 3) \). We are free to choose \( d \) to force exactness for additional monomials. However, it is not possible to get exactness for all fourth degree polynomials. We summarize

CR4. \( L(f) = \frac{1}{4}f(\frac{1}{2},\frac{1}{2}) + \frac{2}{3}(f(0,0) + f(0,\frac{1}{2}) + f(\frac{1}{2}, 0) + f(\frac{1}{2},1) + f(1,\frac{1}{2})) \) is exact for all polynomials of degree \( \leq 3 \). Note that \( L(f) \) is also exact for \( x^3y \) and \( xy^3 \), but not for all polynomials of degree \( \leq 4 \).

Remark 7. It is not possible to choose \( d \) so that \( \lambda = 0 \), since \( 6d^2 - 6d + 2 \) has no real roots.

Remark 8. For the \( n \) cube in general, \( n \geq 3 \), the natural extension would be to use the center of mass of the faces of \( C_n \) to generate \( T(f) \). We leave the details to the reader.

Remark 9. Since \( C_n = [0,1] \times \cdots \times [0,1] \), one could also use Simpson’s rule as a product rule. However, this does not yield any of the rules obtained in this section.

3.2. Connection with interpolation

In this section we investigate whether the cubature rules derived above for the unit square arise by integrating a unique polynomial interpolant to \( f(x,y) \). First, we try a polynomial of the form

\[
p(x,y) = A_1x^2 + A_2y^2 + A_3x + A_4y + A_5.
\]

Given \( 0 \leq a \leq 1, \ 0 \leq b \leq 1, \ 0 \leq c \leq 1, \ 0 \leq d \leq 1, \) and \( f(x,y) \), let \( P_1 = (a,0), \ P_2 = (0,b), \ P_3 = (c,1), \ P_4 = (1,d), \) \( P_5 = (\frac{1}{2}, \frac{1}{2}) \). We wish to choose the \( A_i \) so that \( p(P_k) = f(P_k) \), \( k = 1, \ldots, 5 \). For CR4, let \( a = \frac{1}{2}, \ b = \frac{1}{2}, \ c = \frac{1}{2}, \ d = \frac{1}{2} \). Then the corresponding linear system has the unique solution

\[
\begin{pmatrix}
A_1 \\
A_2 \\
A_3 \\
A_4 \\
A_5
\end{pmatrix} =
\begin{pmatrix}
2b_2 + 2b_4 - 4b_5 \\
2b_1 + 2b_3 - 4b_5 \\
-3b_2 - b_4 + 4b_5 \\
-3b_1 - b_3 + 4b_5 \\
b_1 + b_2 - b_5
\end{pmatrix},
\]
where $b_j = f(P_j)$, $j = 1, \ldots, 5$. It then follows that
\[
\int_0^1 \int_0^1 (A_1 x^2 + A_2 y^2 + A_3 x + A_4 y + A_5) \, dx \, dy = \frac{1}{3} (A_1 + A_2) + \frac{1}{2} (A_3 + A_4) + A_5
\]
\[
= \frac{1}{3} f(\frac{1}{2}, \frac{1}{2}) + \frac{1}{6} (f(0, 0) + f(0, 1) + f(1, 1)),
\]
which is CR4. Thus CR4 does arise as the integral of a unique interpolant of the form $p(x, y)$.

If $a = 1$, $b = 0$, $c = 0$, $d = 1$, however, then the interpolant of the form $p(x, y)$ is not unique.

It is also natural to ask whether our generalization of the Trapezoidal rule, $T(f) = \frac{1}{2} \sum_{k=1}^{4} f(P_k)$, equals the integral of a unique second degree interpolant to $f$ of the form $p(x, y)$ is not unique. For CR3 and CR4 we let $a = b = c = d = \frac{1}{2}$, or $a = 1$, $b = 0$, $c = 0$, $d = 1$. In either case, the interpolant, $p(x, y)$, is not unique.

4. Polygons in the plane

We have already discussed cubature formulas over triangles as a special case of the $n$ simplex, and with points on the boundary other than the vertices. We also discussed cubature formulas over the unit square, as a special case of the $n$ cube, and with points on the boundary other than the vertices. If $n > 4$, and $T(f)$ is generated using the vertices, then the weighted combination $\lambda M(f) + (1 - \lambda) T(f)$ is a poor CR. We examine the special case $n = 6$.

4.1. Six sided regular polygons

Let $D$ be the regular hexagon with vertices $P_1 = (1 + \sqrt{3}, 0)$, $P_2 = (1, 1)$, $P_3 = (-1, 1)$, $P_4 = (-1 - \sqrt{3}, 0)$, $P_5 = (-1, -1)$, $P_6 = (1, -1)$. Then the center of mass of $D = (0, 0)$. We list some useful integrals: $\int_D f(x, y) \, dA = 0$ for any monomial $f$ of degree $\leq 3$, except $\text{Area}(D) = \int_D dA = 4 + 2\sqrt{3}$, $\int_D x^2 \, dA = \frac{16}{3} + 3\sqrt{3}$, $\int_D y^2 \, dA = \frac{4}{3} + \frac{1}{3} \sqrt{3}$. Let $M(f) = (4 + 2\sqrt{3}) f(0, 0)$, $T(f) = (4 + 2\sqrt{3}) \frac{1}{6} \sum_{j=1}^{6} f(P_j)$, $L_4(f) = \lambda M(f) + (1 - \lambda) T(f)$. It follows easily that $L_4$ is exact for $1, x, y$, for any $\lambda$. Now $L_4(x^2) = (4 + 2\sqrt{3})(\frac{1}{6} - \frac{1}{\sqrt{3}})((1 + \sqrt{3})^2 + 4 + (-1 - \sqrt{3})^2)$, and $L_4(y^2) = 4(4 + 2\sqrt{3})(\frac{1}{6} - \frac{1}{\sqrt{3}})$. To make $L_4$ exact for $y^2$, say, we need $4(4 + 2\sqrt{3})(\frac{1}{6} - \frac{1}{\sqrt{3}}) = \frac{4}{3} + \frac{1}{3} \sqrt{3}$, $\lambda = \frac{4 + 3\sqrt{3}}{4 + 3\sqrt{3}}$. But then $L_4(x^2) = (4 + 2\sqrt{3})(\frac{1}{6} - \frac{1}{\sqrt{3}})((1 + \sqrt{3})^2 + 4 + (-1 - \sqrt{3})^2) = \frac{4}{3} + \frac{1}{3} \sqrt{3}$. Hence $L_4$ is only exact for the class of linear polynomials. The following question naturally arises: What if one uses points other than the vertices to generate $T(f)$? Is it possible to obtain degree of exactness equal to two or even three? What about regular polygons in general?

5. Irregular quadrilaterals

Let $D \subset \mathbb{R}^2$ be the trapezoid with vertices $\{(0, 0), (1, 0), (0, 1), (1, 2)\}$ (call them $P_j$).
\[
\int_D dA = \frac{5}{2}, \quad \int_D x \, dA = \frac{5}{6}, \quad \int_D y \, dA = \frac{7}{6} \Rightarrow \text{center of mass of } D \text{ is } (\frac{5}{3}, \frac{7}{3}).
Define the linear functionals

\[ M(f) = \text{Area}(D)f(\frac{5}{7}, \frac{7}{9}) = \frac{3}{7}f(\frac{5}{7}, \frac{7}{9}), \]

\[ T(f) = \text{Area}(D) \left( \frac{1}{4} \sum_{j=1}^{4} f(P_j) \right) = \frac{3}{8}(f(0,0) + f(1,0) + f(0,1) + f(1,2)) \]

and for fixed \( \lambda \), \(0 \leq \lambda \leq 1\),

\[ L_\lambda = \lambda M(f) + (1-\lambda)T(f). \]

To make \( L_\lambda \) exact for \( x \), we have \( L_\lambda(x) = \frac{1}{12}\lambda + \frac{3}{4} = \frac{5}{6} \Rightarrow \lambda = 1 \). Then \( L_\lambda(y) = \frac{1}{24}\lambda + \frac{9}{8} = \frac{7}{6} \). However, \( L_\lambda(xy) = \frac{35}{54} \neq \int_0^1 \int_0^{x+1} xy \, dy \, dx = \frac{17}{24} \). So using the vertices of \( \partial(D) \) for \( T(f) \) only gives exactness for linear functions in general.

**Remark 10.** It is interesting to note that there are no weights \( w_1, w_2, w_3, w_4, w_5 \) such that the CR \( L(f) = w_1 f(\frac{5}{7}, \frac{7}{9}) + w_2 f(0,0) + w_3 f(1,0) + w_4 f(0,1) + w_5 f(1,2) \) is exact for all polynomials of degree \( \leq 2 \).

### 5.1. Other points on boundary of trapezoid

We will try using other points on \( \partial(D) \) to generate \( T(f) \) — say \((a,0),(0,b),(1,c),(d,d+1), \) with \(0 \leq a \leq 1\), \(0 \leq b \leq 1\), \(0 \leq c \leq 2\), \(0 \leq d \leq 1\). Then

\[ L_\lambda(f) = \lambda \frac{3}{2}f(\frac{5}{7}, \frac{7}{9}) + (1-\lambda)\frac{3}{8}(f(a,0) + f(1,c) + f(0,b) + f(d,d+1)). \]

Setting \( L_\lambda(f) = \int_D f \, dA \) for each monomial of degree \( \leq 2 \) yields the following system: \( \frac{3}{2}\lambda + \frac{3}{8}(1-\lambda)(a+1+d) = \frac{5}{6} \), \( \frac{7}{8}\lambda + \frac{3}{8}(1-\lambda)(c + b + d + 1) = \frac{7}{6} \), \( \frac{15}{54}\lambda + \frac{3}{8}(1-\lambda)(c + d(d + 1)) = \frac{17}{24} \), \( \frac{25}{54}\lambda + \frac{3}{8}(1-\lambda)(a^2 + 1 + d^2) = \frac{7}{12} \), \( \frac{49}{54}\lambda + \frac{3}{8}(1-\lambda)(c^2 + b^2 + (d + 1)^2) = \frac{5}{4} \). We used Maple to find the Grobner basis

\[ \{392\lambda - 163, 9a + 9d - 11, 81b - 99d + 20, 180d - 191 + 81c, -22671d + 6583 + 18549d^2 \}. \]

The last equation has solutions \( d = \frac{11}{18} \pm \frac{1}{458} \sqrt{3893} \). Using \( d = \frac{11}{18} + \frac{1}{458} \sqrt{3893} \) and solving the other equations yields

CR5. Let \( a = \frac{11}{18} - \frac{1}{458} \sqrt{3893} \), \( b = \frac{1}{2} + \frac{1}{4122} \sqrt{3893} \), \( c = 1 - \frac{40}{2967} \sqrt{3893} \), \( d = \frac{11}{18} + \frac{1}{458} \sqrt{3893} \), and \( \lambda = \frac{163}{392} \). Then \( L(f) = \lambda \frac{3}{2}f(\frac{5}{7}, \frac{7}{9}) + (1-\lambda)\frac{3}{8}(f(a,0) + f(1,c) + f(0,b) + f(d,d+1)) \) is exact for all polynomials of degree \( \leq 2 \).

Note that \( L(x^3) = 336001/762048 \approx 0.44092 \), while \( I(x^3) = 9/20 = 0.45 \). So \( L \) is not exact for all cubics. It is natural to ask whether one can obtain degree of exactness two for any trapezoid in the plane?

### 6. Unit disc

In this section we consider a regular polygon with an infinite number of sides, the unit disc \( D \). The \( n \) roots of unity \( z_k = e^{2\pi ik/n}, k = 1, \ldots, n \), can be used to generate \( T(f) = (\pi/n) \sum_{k=1}^{n} f(\cos(2\pi k/n), \sin(2\pi k/n)) \).
\[ \sin(2\pi k/n) \]. Since the center of mass of \( D = (0, 0) \) and \( \text{area}(D) = \pi \), the analogy of our formulas for the triangle and the square is \( M(f) = \pi f(0,0), \ L(f) = \lambda \pi f(0,0) + (1 - \lambda) \frac{\pi}{n} \sum_{k=1}^{n} f(\cos(2\pi k/n, \sin(2\pi k/n)) \). It is not hard to show, however, that the only good choice is \( n = 4 \). This gives the formulas
\[ L(f) = \lambda \pi f(0,0) + (1 - \lambda) \frac{\pi}{4} f(1,0) + f(0,1) + f(-1,0) + f(0,-1). \]

We list the following integrals without proof:

If \( m \) and \( n \) are even whole numbers, then
\[ \int_{D} x^{m}y^{n} dA = \frac{\pi}{m+n+2} \left( \frac{(n-1)!(m-1)!}{2^{m+n-3}((n/2) - 1)!(m/2 - 1)!(m+n)/2!} \right). \]

If \( m \) is an even whole number and \( n = 0 \), then
\[ \int_{D} x^{m}y^{n} dA = \frac{\pi}{m+2} \left( \frac{(m-1)!}{2^{m-2}((m/2) - 1)!(m/2)!} \right). \]

If \( n \) is an even whole number and \( m = 0 \), then
\[ \int_{D} x^{m}y^{n} dA = \frac{\pi}{n+2} \left( \frac{(n-1)!}{2^{n-2}((n/2) - 1)!(n/2)!} \right). \]

If \( m \) and/or \( n \) is an odd whole number, then \( \int_{D} x^{m}y^{n} dA = 0 \). It is then easy to prove that the choice \( \lambda = \frac{1}{2} \) gives
\( \text{CR6. } L(f) = (\pi/2) f(0,0) + (\pi/8)(f(1,0) + f(0,1) + f(-1,0) + f(0,-1)) \) is exact for all polynomials of degree \( \leq 3 \).

7. Summary of cubature rules

These are the CRs we derived as a generalization of Simpson’s rule for functions of one variable. If \( D_{n} \) is a polygonal region in \( \mathbb{R}^{n} \), let \( P_{0}, \ldots, P_{m} \) denote the \( m+1 \) vertices of \( D_{n} \) and \( P_{m+1} \) the center of mass of \( D_{n} \). The generalization is based on the weighted combination \( L = \lambda M(f) + (1 - \lambda) T(f) \), where \( M(f) = \text{Vol}(D_{n})f(P_{m+1}), \ T(f) = \text{Vol}(D_{n})[(1/(m + 1)] \sum_{j=0}^{m} f(P_{j}) \). Unless noted otherwise, each of the rules has the following properties: All of the weights are positive, and all but one of the weights are equal. All of the knots lie inside the region of integration, and all but one of the knots lies on the boundary of the region. Note that it is desirable to have as many knots as possible on \( \partial(D_{n}) \) if one subdivides the region and compounds the CR.

7.1. \( n \) Simplex \( T_{n} \)

- Using the vertices,
\[ L(f) = \frac{n+1}{(n+2)m!} f(P_{n+1}) + \frac{1}{(n+2)!} \sum_{j=0}^{n} f(P_{j}) \]
is exact for all polynomials of degree \( \leq 2 \).
Letting \( \{Q_k\} \) denote the center of mass of the faces of \( T_n \),

\[
L(f) = -(n - 2)^n + \frac{1}{n + 2} n! f(1/(n + 1), \ldots, 1/(n + 1)) + \frac{n^2}{(n + 2)!} \sum_{k=1}^{n+1} f(Q_k)
\]

is exact for all polynomials of degree \( \leq 2 \). All but one weight is positive if \( n > 2 \).

7.2. Unit \( n \) cube \( C_n \)

- **General** \( n \): Let \( P_0, \ldots, P_{m-1} \) denote the \( m \) vertices of \( C_n \), \( m = 2^n \). Then

\[
L(f) = \frac{2}{3} f \left( \frac{1}{2}, \ldots, \frac{1}{2} \right) + \frac{1}{3} \frac{1}{2^n} \sum_{j=0}^{2^n-1} f(P_j)
\]

is exact for all polynomials of degree \( \leq 3 \).

- \( n = 2 \): \( L(f) = \frac{1}{2} f \left( \frac{1}{2}, \frac{1}{2} \right) + \frac{1}{6} (f(1,0) + f(0,1) + f(1,1) + f(1,0)) \) is exact for all polynomials of degree \( \leq 3 \).

7.3. Unit disc \( D \)

\[
L(f) = (\pi/2)f(0,0) + (\pi/8)(f(1,0) + f(0,1) + f(-1,0) + f(0,-1))
\]

is exact for all polynomials of degree \( \leq 3 \).

7.4. A trapezoid in the plane

Let \( D \subset \mathbb{R}^2 \) be the trapezoid with vertices \( \{(0,0), (1,0), (0,1), (1,2)\} \).

Let \( a = \frac{11}{18} - \frac{1}{458} \sqrt{3893} \approx 0.47488 \), \( b = \frac{1}{2} + \frac{11}{4122} \sqrt{3893} \approx 0.6665 \), \( c = 1 - \frac{10}{2061} \sqrt{3893} \approx 0.69726 \), \( d = \frac{11}{18} + \frac{1}{458} \sqrt{3893} \approx 0.74734 \), and \( \lambda = \frac{163}{392} \approx 0.41582 \). Then

\[
L(f) = \lambda \frac{3}{8} f \left( \frac{5}{8}, \frac{5}{8} \right) + (1 - \lambda) \frac{3}{8} (f(a,0) + f(1,c) + f(0,b) + f(d,d+1))
\]

is exact for all polynomials of degree \( \leq 2 \).

References