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## Numerical Quadrature

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- When you took calculus, you quickly discovered that integration is much more difficult than differentiation. In fact, the majority of integrals can not be integrated analytically. For example, integrals such as

$$\int_a^b \sin x^2 dx \quad \int_a^b e^{-x^2} dx$$

can not be integrated exactly.

- Other integrals may be defined over higher dimensional spaces with complicated boundaries.
- In addition, sometimes we may only know the integrand at a set of points.
- Sometimes we can represent the integrand as an infinite series but even if we can integrate each term of the series exactly we must still truncate the series and thus approximate the integral.

For a function of one independent variable, the basic idea of a quadrature rule is to replace the definite integral by a sum of the integrand evaluated at certain points (called **quadrature points** ) multiplied by a number (called **quadrature weights** ).

$$\int_a^b f(x) dx \approx w_1 f(q_1) + w_2 f(q_2) + \cdots + w_n f(q_n) = \sum_{i=1}^n f(q_i) w_i$$

where the  $w_i$  are weights and the  $q_i$  are quadrature points and  $n$  is the number of quadrature points.

For example, for the **left Riemann sum rule**

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

we have  $n = 1$ ,  $q_1 = a$  and  $w_1 = (b - a)$ .

## Goals:

- To investigate Newton-Cotes formulas for approximating integrals in  $\mathbb{R}^1$ .
- To investigate Gauss quadrature formulas for approximating integrals in  $\mathbb{R}^1$ .
- To determine the highest degree of polynomial that the quadrature rule integrates exactly (the degree of precision)
- To estimate the error we make in using quadrature rules.
- To investigate piecewise integration (as we did for piecewise interpolation).
- To look at approximating improper integrals and integrals with singularities.
- To extend some of our results in one dimension to integrals in higher dimensions.
- In the lab you will investigate adaptive quadrature and nested rules.

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## Newton-Cotes Quadrature Formulas

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The idea behind Newton-Cotes formulas is to use **evenly spaced** quadrature points so that we have “nice” points. We then interpolate these quadrature points and integrate to get the weights. Thus Newton-Cotes formulas are **interpolatory quadrature rules**. There are two basic types of Newton-Cotes formulas:

**open type:** doesn't use the endpoints of the interval as quadrature points and

**closed type:** uses the endpoints of the interval as quadrature points

Once you choose the number of points in your Newton-Cotes formula and decide whether to use an open or closed formula then all that remains is to determine the weights  $w_i$ . To do this we simply use a Lagrange polynomial to interpolate  $f(x)$  at the quadrature points. We then use this polynomial to approximate  $f(x)$  and integrate it exactly. We will get a sum of terms where  $f$  is evaluated at quadrature point times a number; this number is the weight for that quadrature point. This is the reason that Newton-Cotes quadrature rules are called interpolatory.

The simplest open Newton-Cotes quadrature formula is the **Midpoint Rule** where

$$\text{Midpoint Rule: } \int_a^b f(x) dx \approx (b - a) f\left(\frac{a + b}{2}\right)$$

Here the quadrature point  $q_1 = (a + b)/2$  is the midpoint of  $[a, b]$  and the weight is  $w_1 = b - a$ , the length of the interval. The midpoint rule is a **one point rule** because it only has one quadrature point. Note that if  $f(x) \geq 0$  for  $a \leq x \leq b$  then we are approximating the integral by the area of the rectangle with base  $b - a$  and height  $f\left(\frac{a+b}{2}\right)$ .

We can derive this formula by approximating  $f(x)$  on  $[a, b]$  by  $f$  evaluated at the quadrature point, i.e.,  $f\left(\frac{a+b}{2}\right)$  (the constant Lagrange interpolating polynomial) and integrating this to get an approximation to  $\int_a^b f(x) dx$ , i.e.,

$$\int_a^b f\left(\frac{a + b}{2}\right) dx = (b - a) f\left(\frac{a + b}{2}\right)$$

Consequently our weight is determined to be  $b - a$ .

The simplest closed Newton-Cotes formula is the **Trapezoidal Rule** which is a two

point rule because we use the two endpoints  $x = a, b$ . To determine the weights we fit a linear polynomial (i.e., a line) through the two points.

We have the linear Lagrange polynomial through  $(a, f(a))$  and  $(b, f(b))$

$$p_1(x) = \frac{f(b) - f(a)}{b - a}(x - a) + f(a)$$

which we use to approximate  $f(x)$ . Integrating we get

$$\begin{aligned} \int_a^b f(x) dx &\approx \int_a^b p_1(x) dx = \left( \frac{f(b) - f(a)}{b - a} \right) \frac{(x - a)^2}{2} \Big|_a^b + x f(a) \Big|_a^b \\ &= \left( \frac{f(b) - f(a)}{b - a} \right) \left[ \frac{(b - a)^2}{2} - 0 \right] + f(a)(b - a) = (b - a) \frac{f(a) + f(b)}{2} \end{aligned}$$

Thus the weights are  $w_1 = w_2 = (b - a)/2$ .

The rule gets its name because the area of the trapezoid with base  $b - a$  is just

$$(b - a)f(a) + \frac{1}{2}(b - a)(f(b) - f(a)) = (b - a) \frac{f(a) + f(b)}{2}.$$

Thus, if  $f(x) \geq 0$  for  $a \leq x \leq b$  then we are approximating the area under the curve  $f(x)$  between  $x = a$  and  $x = b$  by a trapezoid.

**Closed Trapezoid Rule:** 
$$\int_a^b f(x) dx \approx (b - a) \frac{f(a) + f(b)}{2}$$

Oftentimes the Midpoint Rule is considered both an open and closed Newton-Cotes rule; we will use this fact in the lab.

Of course, the next closed rule would use three points; since it is closed and we use evenly spaced points, then we choose the endpoints and the midpoint of the interval. To determine the weights we first obtain the quadratic Lagrange interpolating polynomial which passes through  $(a, f(a))$ ,  $(\frac{a+b}{2}, f(\frac{a+b}{2}))$ , and  $(b, f(b))$  which is

$$p_2(x) = f(a) \frac{(x - \frac{a+b}{2})(x - b)}{(a - \frac{a+b}{2})(a - b)} + f\left(\frac{a+b}{2}\right) \frac{(x - a)(x - b)}{(\frac{a+b}{2} - a)(\frac{a+b}{2} - b)} + f(b) \frac{(x - a)(x - \frac{a+b}{2})}{(b - \frac{a+b}{2})(b - a)}$$

If  $h = b - a$  then we have

$$p_2(x) = \frac{2f(a)}{h^2} \left(x - \frac{a+b}{2}\right)(x-b) - \frac{4f\left(\frac{a+b}{2}\right)}{h^2} (x-a)(x-b) + \frac{2f(b)}{h^2} (x-a)\left(x - \frac{a+b}{2}\right)$$

Thus

$$w_1 = \frac{2}{h^2} \int_a^b \left(x - \frac{a+b}{2}\right)(x-b) dx = \frac{2}{h^2} \frac{h^3}{12} = \frac{h}{6}$$

Similarly  $w_2 = \frac{2h}{3}$  and  $w_3 = \frac{h}{6}$ .

**Simpson's Rule:** 
$$\int_a^b f(x) dx \approx \frac{b-a}{6} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

So far for closed rules we have the two-point Trapezoidal Rule and the three-point Simpson's Rule. In the table where we summarize Newton-Cotes formulas we list the next rule which is called Simpson's 3/8 Rule which you will explore in the exercises.

For open rules we have just derived the Midpoint Rule which is a one-point rule. The next would be a two-point Rule using the points  $a + (b-a)/3$  and  $a + 2(b-a)/3$ . This also forms a trapezoid to approximate the area so it is called an open trapezoid rule. You will explore this method in the exercises.



We can continue in this manner by choosing to use more quadrature points and generate both open and closed Newton-Cotes families of quadrature rules. Before we tabulate the rules we look at the degree of precision of each rule and the error.

## Degree of Precision for Quadrature Rules

One way to compare quadrature rules is to determine the highest degree polynomial that the rule integrates exactly, that is, the degree of precision of the rule.

The **Midpoint Rule integrates a linear function exactly** but not a quadratic. To see this we first integrate a linear and quadratic polynomial exactly to get:

$$\int_a^b (a_0 + a_1x) dx = \left( a_0x + a_1\frac{x^2}{2} \right) \Big|_a^b = a_0(b-a) + \frac{a_1}{2}(b^2 - a^2)$$

$$\int_a^b (a_0 + a_1x + a_2x^2) dx = \left( a_0x + a_1\frac{x^2}{2} + a_2\frac{x^3}{3} \right) \Big|_a^b = a_0(b-a) + \frac{a_1}{2}(b^2 - a^2) + \frac{a_2}{3}(b^3 - a^3)$$

Applying the midpoint rule to a general linear function  $f(x) = a_0 + a_1x$  gives

$$\int_a^b f(x) dx \approx (b-a)f\left(\frac{a+b}{2}\right) = (b-a)\left(a_0 + a_1\left(\frac{a+b}{2}\right)\right) = (b-a)a_0 + \frac{a_1}{2}(b^2 - a^2)$$

which agrees with the result above. However, applying the midpoint rule to a quadratic polynomial does not give the correct answer

$$(b-a)\left(a_0 + a_1\left(\frac{a+b}{2}\right) + a_2\left(\frac{a+b}{2}\right)^2\right) \neq a_0(b-a) + \frac{a_1}{2}(b^2 - a^2) + \frac{a_2}{3}(b^3 - a^3)$$

Because the Trapezoid Rule uses two quadrature points whereas the Midpoint Rule only uses one; we might think that its degree of precision would be higher. However, it only integrates linear polynomials since applying the rule to  $f(x) = a_0 + a_1x$  gives

$$(b-a)\frac{[a_0 + a_1a] + [a_0 + a_1b]}{2} = (b-a)a_0 + \frac{a_1}{2}(b^2 - a^2) = \int_a^b (a_0 + a_1x) dx$$

but applying the rule to  $f(x) = a_0 + a_1x + a_2x^2$  gives

$$(b-a)\frac{[a_0 + a_1a + a_2a^2] + [a_0 + a_1b + a_2b^2]}{2} = (b-a)a_0 + \frac{a_1}{2}(b^2 - a^2) +$$

$$\begin{aligned}
& +\frac{a_2}{2} (b^3 - a^3 + a^2b - ab^2) \neq a_0(b - a) + \frac{a_1}{2}(b^2 - a^2) + \frac{a_2}{3}(b^3 - a^3) \\
& = \int_a^b (a_0 + a_1x + a_2x^2)dx
\end{aligned}$$

If we do the math we can demonstrate that Simpson's rule integrates polynomials of degree three exactly; this will be clear when we look at the error estimate.

If we take the Midpoint Rule as the one-point closed (as well as open) Newton-Cotes formula then what we have seen is that for closed rules the one-point rule has degree of precision one, the two-point rule has degree of precision one and the three point rule has degree of precision three. For Newton-Cotes rules this is true, in general.

**Newton-Cotes**  $N$  even - degree of precision  $N - 1$  &  $N$  odd - degree of precision  $N$

## Computing the Error in an Integration Rule

We first compute the error for the Midpoint Rule:

$$E_{\text{midpt}} = \left| \int_a^b f(x) dx - (b-a)f\left(\frac{a+b}{2}\right) \right|$$

In order to simplify this expression we can expand  $f((a+b/2))$  in a Taylor series but then we need to represent the integral in terms of  $f(a)$  and its derivatives. From the Fundamental Theorem of Calculus we know there is a function  $F(x)$  such that

$$\int_a^x f(s) ds = F(x),$$

so that  $F(b)$  is our desired integral. Now we expand  $F(a+h) = F(b)$  using a Taylor's series with remainder to get

$$\int_a^{a+h} f(s) ds = F(a+h) = F(a) + F'(a)h + F''(a)\frac{h^2}{2} + F'''(a)\frac{h^3}{6} + \mathcal{O}(h^4)$$

where we have set  $h = b - a$ . Now from the definition of  $F(x)$ , we have that

$F(a) = 0$ ,  $F'(a) = f(a)$ ,  $F''(a) = f'(a)$  so that

$$\int_a^{a+h} f(s) ds = 0 + f(a)h + f'(a)\frac{h^2}{2} + f''(a)\frac{h^3}{6} + \mathcal{O}(h^4)$$

To combine this with the Midpoint Rule we expand  $f\left(\frac{a+b}{2}\right) = f\left(a + \frac{h}{2}\right)$  in a Taylor's series about  $x = a$

$$hf\left(a + \frac{h}{2}\right) = h \left[ f(a) + \frac{h}{2}f'(a) + \frac{h^2}{2 \cdot 4}f''(a) + \frac{h^3}{6 \cdot 8} + \mathcal{O}(h^3) \right]$$

Combining these results gives the final error

$$E_{\text{midpt}} = \left| \int_a^b f(x) dx - hf\left(\frac{a+b}{2}\right) \right| = f''(a)\frac{h^3}{24} = \mathcal{O}(h^3)$$

Recall that the Midpoint Rule integrates linear functions exactly but not quadratic functions; this is clear from the error estimate because the second derivative of a linear function is zero whereas the second derivative of a quadratic is not zero, in general.

Recall that the Trapezoid Rule uses two quadrature points so we might expect its error to be smaller than the Midpoint Rule which just used one point. However, this is not the case, as we shall see.

$$E_{\text{trap}} = \left| \int_a^b f(x) dx - (b-a) \frac{f(a) + f(b)}{2} \right|$$

As before, we let

$$\int_a^x f(s) ds = F(x)$$

and expand using a Taylor's series with remainder, and use the definition of  $F(x)$  to get

$$\int_a^{a+h} f(s) ds = 0 + f(a)h + f'(a)\frac{h^2}{2} + f''(a)\frac{h^3}{6} + \mathcal{O}(h^4)$$

To combine this with the Trapezoid Rule we only need to expand  $f(b)$  since the other term involves  $f(a)$ . To this end we have

$$f(b) = f(a+h) = f(a) + f'(a)h + \frac{h^2}{2}f''(a) + \frac{h^3}{6}f'''(a) + \mathcal{O}(h^4)$$

Combining these results gives the final error

$$E_{\text{trap}} = \left| \int_a^b f(x) dx - h \frac{f(a) + f(b)}{2} \right| = \left| f(a)h + f'(a)\frac{h^2}{2} + f''(a)\frac{h^3}{6} + \mathcal{O}(h^4) \right|$$

$$-\frac{h}{2} \left( f(a) + \left[ f(a) + f'(a)h + \frac{h^2}{2}f''(a) + \frac{h^3}{6}f'''(a) + \mathcal{O}(h^4) \right] \right) |$$

$$= \left| f''(a)\frac{h^3}{12} + \mathcal{O}(h^4) \right| = \mathcal{O}(h^3)$$

So from this estimate you can see that the Midpoint Rule and the Trapezoid Rule are both  $\mathcal{O}(h^3)$  and because the error estimate involves the second derivative, they are exact for linear polynomials but not quadratic polynomials and thus their degree of precision is one.

To determine the error in Simpson's rule we must expand both  $f(a + \frac{h}{2})$  and  $f(b) = f(a + h)$  in the formula in Taylor's series. Completing this gives an error for Simpson's method of

$$E_{\text{Simp}} = \frac{h^5}{180} f''''(\xi) = \mathcal{O}(h^5)$$

This says that the degree of precision of Simpson's method is three, i.e., it integrates cubic polynomials exactly; this is due to the fact that the fourth derivative of a cubic is zero but the fourth derivative of a quartic is not.

We tabulate some of the open and closed Newton-Cotes Formulas below. For

brevity we use  $h = b - a$  and  $f_i$  to denote  $f(x)$  evaluated at the  $i$ th quadrature point.



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## Open Newton-Cotes Formulas

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Method	Quad Pts	Formula	Degree of Precision	Error Term
Midpoint	$a + \frac{h}{2}$	$hf_1$	1	$\frac{h^3}{24} \max_{\xi \in [a,b]}  f''(\xi) $
Trapezoid	$a + \frac{h}{3}, a + \frac{2h}{3}$	$\frac{h}{2} (f_1 + f_2)$	1	$\frac{h^3}{36} \max_{\xi \in [a,b]}  f''(\xi) $
Milne's rule	$a + \frac{h}{4}, a + \frac{h}{2},$ $a + \frac{3h}{4}$	$\frac{h}{3} (2f_1 - f_2 + 2f_3)$	3	$\frac{7h^5}{23040} \max_{\xi \in [a,b]}  f''''(\xi) $

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## Closed Newton-Cotes Formulas

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Method	Quad Pts	Formula	Degree of Precision	Error Term
Trapezoid	$a, b$	$\frac{h}{2} (f_1 + f_2)$	1	$\frac{h^3}{12} \max_{\xi \in [a,b]}  f''(\xi) $
Simpson's	$a, a + \frac{h}{2}, b$	$\frac{h}{6} (f_1 + 4f_2 + f_3)$	3	$\frac{h^5}{180} \max_{\xi \in [a,b]}  f''''(\xi) $
3/8 rule	$a, a + \frac{h}{3}, a + \frac{2h}{3}, b$	$\frac{h}{8} (f_1 + 3f_2 + 3f_3 + f_4)$	3	$\frac{h^5}{6480} \max_{\xi \in [a,b]}  f''''(\xi) $

Higher order formulas can be found on Wikipedia.

## Example

Let's take as an example an integral that we can integrate exactly so we can compute the exact error and show that it agrees with our theoretical results.

$$\int_0^{.6} x^4 dx = 0.015552$$

Here  $f(x) = x^4$ . We apply our three open Newton-Cotes rules with  $h = 0.6$ .

(I) Midpoint Rule: one quadrature point 0.3

$$\int_0^{.6} x^4 dx \approx 0.6(0.3)^4 = .00486$$

with an error of  $E_{\text{mid}} = 0.010692 = 1.0692 \cdot 10^{-2}$ . The theoretical error bound is  $.6^3/24 \max |f''(x)|$  where  $f''(x) = 12x^2$  which is an increasing function on  $[0, .6]$  so its maximum value there is  $12(.6)^2$ . Therefore the theoretical error bound is  $(.6^3/24)12(.6)^2 = 0.038888$  and clearly our error is smaller than this.

(II) Open Trapezoid Rule: two quadrature points 0.2, 0.4

$$\int_0^{.6} x^4 dx \approx \frac{0.6}{2} [(0.2)^4 + (0.4)^4] = 0.00816$$

with an error of  $E_{\text{trap}} = 0.007392 = 7.392 \cdot 10^{-3}$ . The theoretical error is  $.6^3/36 \max |f''(x)| = (.6^3/36)12(.6)^2 = 0.0039539$

(III) Milne Rule: three quadrature points 0.15, 0.3, and 0.45

$$\int_0^{.6} x^4 dx \approx \frac{0.6}{3} [2(0.15)^4 - (0.3)^4 + 2(0.45)^4] = 0.014985$$

with an error of  $E_{\text{milne}} = 0.000567 = 5.67 \cdot 10^{-4}$ . The theoretical error bound is  $7(.6)^5/23040 \max |f''''| = 7(.6)^5/23040 \cdot 24 = 0.000567$ . Note that here the theoretical bound matches the exact error because the maximum value of  $f''''$  on  $[0, .6]$  is a constant so there is no estimate as in the other cases.

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## Composite Integration Rules

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If we approximate our integral using the Midpoint rule and are unhappy with the size of the error, then our only option at this point is to apply a more accurate method. However, as we keep increasing the number of quadrature points, we need a higher degree Lagrange interpolating polynomial and we have seen that there is typically not a good choice. Similar to when we used piecewise interpolation we can divide our interval into subintervals and apply a lower order rule over each subinterval. These are called **composite rules**.

First we look at the **Composite Midpoint Rule**. As before, assume we want to integrate

$$\int_a^b f(x) dx$$

So we take the interval  $[a, b]$  and divide it into  $M$  subintervals of length  $\frac{b-a}{M}$ .

Then we apply the Midpoint Rule over each interval. The quadrature points are

$$q_1 = a + \frac{b-a}{2M}, \quad q_2 = q_1 + \frac{b-a}{M} \quad q_3 = q_1 + 2\frac{b-a}{M}, \quad \dots \quad q_M = q_1 + (M-1)\frac{b-a}{M}$$

$$\int_a^b f(x) dx \approx \frac{b-a}{M} [f(q_1) + f(q_2) + \dots + f(q_M)] = \frac{b-a}{M} \sum_{i=1}^M f(q_i)$$

As an example for a closed Newton-Cotes formula we use the composite Trapezoid Rule which is  $h/2$  times the average of  $f(x)$  at the endpoints. Using  $M$  subintervals of length  $\frac{b-a}{M}$  we apply the Trapezoid Rule over each interval. The quadrature points are

$$q_1 = a, \quad q_2 = a + \frac{b-a}{M}, \quad q_3 = q_2, \quad q_4 = q_2 + \frac{b-a}{M}, \quad q_5 = q_4 \dots$$

$$\int_a^b f(x) dx \approx \frac{b-a}{2M} \left[ \left( f(q_1) + f(q_2) \right) + \left( f(q_3) + f(q_4) \right) \right. \\ \left. + \left( f(q_4) + f(q_5) \right) + \dots + \left( f(q_{M-2}) + f(q_{M-1}) \right) + \left( f(q_{M-1}) + f(q_M) \right) \right]$$

$$= \frac{b-a}{2M} \left[ f(q_1) + 2f(q_2) + 2f(q_4) + \cdots + 2f(q_{M-1}) + f(q_M) \right]$$

## Error in Composite Rules

We look at the Composite Midpoint Rule as an example to see how to compute the error. Recall that when we applied the rule on an interval  $[a, b]$  then the error was bounded by

$$E_{\text{midpt}} \leq \frac{(b-a)^3}{24} \max_{x \in [a, b]} |f''(x)|$$

So on each interval of length  $\frac{b-a}{M}$  (assuming  $M$  subintervals) we have an error bound on interval  $I_j$  of

$$\frac{\left(\frac{b-a}{M}\right)^3}{24} \max_{x \in I_j} |f''(x)|$$

Now if we sum these errors up over the  $M$  subintervals  $I_j$  and bound the maximum of  $f''$  over each  $I_j$  by the maximum over all  $[a, b]$  then we have the total

error of

$$\sum_{j=1}^M \frac{(b-a)^3}{24M^3} \max_{x \in I_j} |f''(x)| \leq \frac{(b-a)^3}{24M^2} \max_{x \in [a,b]} |f''(x)|$$

**Example** Apply the composite Midpoint Rule to the integral

$$\int_0^1 x^3 dx = 0.25$$

using  $M = 1, 2, 4, 8$  equal subintervals. Obtain the approximations and the errors. Compare with the theoretical results.

Since  $f(x) = x^3$ ,  $f''(x) = 6x$  then  $\max |f''(x)| = 6$  on  $[0, 1]$ . Using one interval of length one we have

$$\int_0^1 x^3 dx \approx 1[.5^3] = \frac{1}{8} \quad \text{error} \quad 0.125 < \frac{1}{24}6 = 0.25$$

Using two subintervals of length one-half we have

$$\int_0^1 x^3 dx \approx \frac{1}{2} [.25^3 + .75^3] = 0.21875 \quad \text{error} \quad 0.03125 < \frac{6}{4 \cdot 24} = 0.0625$$



Using four subintervals of length one-fourth we have

$$\int_0^1 x^3 dx \approx \frac{1}{4} \left[ \left(\frac{1}{8}\right)^2 + \left(\frac{3}{8}\right)^2 + \left(\frac{5}{8}\right)^2 + \left(\frac{7}{8}\right)^2 \right] = 0.242188$$

$$\text{error } 0.0078125 < 0.015625$$

Using eight subintervals of length one-eighth we have

$$\int_0^1 x^3 dx \approx 0.248047 \quad \text{error } 0.00195313 < 0.00390625$$

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## Gauss-Legendre Quadrature

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In Newton-Cotes formulas we fixed the quadrature points as uniformly spaced in the interval and then an interpolation polynomial was used to determine the weights. We saw that the degree of precision of the formulas was either  $N - 1$  or  $N$  depending on whether the rule was even or odd. One might think that if we let the quadrature points and the weights be unknowns then we could derive a quadrature formula which has a higher degree of precision than Newton-Cotes formulas. Also, when we studied interpolation we saw that other points than uniformly spaced ones often work better such as Chebyshev points.

The most commonly used of these rules is **Gauss-Legendre quadrature** or just **Gauss quadrature**. One way to derive a Gauss rule is to determine the quadrature points and weights such that the rule integrates as high a degree polynomial as possible; i.e., we optimize the rule. Hence the Gauss-Legendre rules are not interpolatory like the Newton-Cotes rules. Another way to derive the quadrature points is to take the roots of the Legendre polynomial. We will see that if we

use  $N$  quadrature points then we can integrate a polynomial of degree  $2N - 1$  exactly with these rules. (Or equivalently, if we use  $N + 1$  quadrature points then we can integrate a polynomial of degree  $2N + 1$  exactly.)

The first Gauss rule is the Midpoint Rule where we use one quadrature point. Note that here  $N = 1$  so from above the Midpoint should have degree of precision  $2N - 1 = 1$  and this agree with what we already know because we have seen that the Midpoint Rule integrates linear polynomials exactly. We will derive a two-point Gauss rule directly and then show that the quadrature points are roots of the Legendre polynomial.

## Derivation of Two-Point Gauss Rule

Let the two quadrature points and weights be  $(q_i, w_i)$ ,  $i = 1, 2$ . Then a two point quadrature rule for an integral  $I$  is of the form

$$I \approx f(q_1)w_1 + f(q_2)w_2$$

so we have four variables and so we can satisfy four different conditions. This means that we should be able to choose the points and weights to integrate a

cubic polynomial exactly. This agrees with our formula because here we are using  $2 = N$  points and we said we can integrate polynomials of degree  $2N - 1 = 3$  exactly with Gauss rules.

We set up the equations to determine the quadrature points and weights by requiring the rule to integrate the cubic  $a_0 + a_1x + a_2x^2 + a_3x^3$  exactly. This means the following relationship must hold:

$$\int_{-1}^1 (a_0 + a_1x + a_2x^2 + a_3x^3) dx = w_1 [a_0 + a_1q_1 + a_2q_1^2 + a_3q_1^3] + \\ + w_2 [a_0 + a_1q_2 + a_2q_2^2 + a_3q_2^3]$$

Integrating gives us

$$\int_{-1}^1 (a_0 + a_1x + a_2x^2 + a_3x^3) dx = 2a_0 + \frac{2a_2}{3}$$

so that

$$2a_0 + \frac{2a_2}{3} = w_1 [a_0 + a_1q_1 + a_2q_1^2 + a_3q_1^3] + w_2 [a_0 + a_1q_2 + a_2q_2^2 + a_3q_2^3]$$

Rearranging this expression yields

$$a_0 [w_1 + w_2 - 2] + a_1 [w_1 q_1 + w_2 q_2] + a_2 [w_1 q_1^2 + w_2 q_2^2] + a_3 \left[ w_1 q_1^3 + w_2 q_2^3 - \frac{2}{3} \right] = 0$$

Now the coefficients  $a_i$ ,  $i = 0, 1, 2, 3$  are arbitrary so they can't be zero so we need to make the terms inside the square brackets to be each zero which will give us the four nonlinear equations for our four unknowns:

$$\begin{aligned} w_1 + w_2 &= 2 \\ w_1 q_1 + w_2 q_2 &= 0 \\ w_1 q_1^2 + w_2 q_2^2 &= \frac{2}{3} \\ w_1 q_1^3 + w_2 q_2^3 &= 0 \end{aligned}$$

We could have gotten the same equations if we had required the rule to integrate a constant,  $x$ ,  $x^2$  and  $x^3$ . Solving these we get

$$w_1 = w_2 = 1 \quad q_1 = -\frac{1}{\sqrt{3}}, \quad q_2 = \frac{1}{\sqrt{3}}$$

So the two point Gauss quadrature rule is

$$\int_{-1}^1 f(x) dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

For a three point Gauss rule we have  $N = 3$  points so we have six unknowns which means we should be able to integrate a fifth degree polynomial exactly. This agrees with the fact that we want to integrate polynomials of degree  $2N - 1$  exactly. We will not derive it here but the approach is the same.

## Legendre Polynomials

Legendre polynomials are solutions to the Legendre ordinary differential equation

$$\frac{d}{dx} \left[ (1 - x^2) \frac{d}{dx} P_n(x) \right] + n(n + 1)P_n(x) = 0$$

and are given by the recursion formula

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} [(x^2 - 1)^n] .$$

Thus

$$P_1(x) = \frac{1}{2} 2x = x,$$

$$P_2(x) = \frac{1}{8} \frac{d^2}{dx^2} (x^4 - 2x^2 + 1) = \frac{1}{8} \frac{d}{dx} (4x^3 - 4x) = \frac{1}{2} (3x^2 - 1), \quad \dots$$

The root of  $P_1(x) = x$  is just  $x = 0$  which is the quadrature point for the Midpoint Rule. The roots of  $P_2 = \frac{1}{2}(3x^2 - 1)$  are just  $x = \pm \frac{1}{\sqrt{3}}$  which are the roots for the two-point Gauss rule that we derived.

In the table below we summarize the first five Gauss quadrature rules.

TABLE 0.1  
Gauss quadrature formulas on  $[-1, 1]$

$n$	nodes	weights
1	0.0000000000	2.0000000000
2	$\pm \frac{1}{\sqrt{3}} = \pm 0.5773502692$	1.0000000000
3	$\pm 0.7745966692$	0.5555555556
	0.0000000000	0.8888888889
4	$\pm 0.8611363116$	0.3478548451
	$\pm 0.3399810436$	0.6521451549
5	$\pm 0.9061798459$	0.2369268850
	$\pm 0.5384693101$	0.4786286701
	0.0000000000	0.5688888889

## Transforming a Gauss rule to an arbitrary interval

Gauss quadrature rules are always given on the interval  $[-1, 1]$  but we need to perform integrations over other intervals.

If the domain of integration is different from  $[-1, 1]$ , then a change of variables is needed. For example, to compute the integral  $\int_a^b f(\hat{x}) d\hat{x}$  we use the linear mapping  $\hat{x} = a + \frac{b-a}{2}(x+1)$  to map to the integral over  $[-1, 1]$ . Note that this mapping sends the point  $x = -1$  to  $\hat{x} = a$  and  $x = 1$  to  $\hat{x} = b$ . Then with this change of variables we have

$$\int_a^b f(\hat{x}) d\hat{x} = \frac{b-a}{2} \int_{-1}^1 f\left(a + \frac{b-a}{2}(x+1)\right) dx,$$

where we have used the fact that  $d\hat{x} = (b-a)/2dx$ . Then we apply the quadrature rule to the integral over  $(-1, 1)$ . Note that we have just modified the quadrature weight in the given rule by  $\frac{b-a}{2}$  and mapped the quadrature point to the interval  $[a, b]$ .



## Example

Approximate  $\int_0^\pi \sin x \, dx = 2$  using a 2-point and a 3-point Gauss quadrature rule. Calculate the error for each rule. Compare your results with using Simpson's rule.

For the 2-point rule we need to transform the points  $x = \pm 1/\sqrt{3}$  to the interval  $[0, \pi]$ . We have the transformed points as

$$0 + \frac{\pi}{2} \left( \pm \frac{1}{\sqrt{3}} + 1 \right) \Rightarrow q_1 = 0.6638966, \quad q_2 = 2.477696$$

and the weights

$$w_1 = w_2 = \frac{\pi}{2}(1)$$

Using these points and weights gives the approximation

$$\int_0^\pi \sin x \, dx \approx \frac{\pi}{2} \sin(0.6638966) + \frac{\pi}{2} \sin(2.477696) = 1.93582$$

giving an error of 0.06418.

For the 3-point rule we need to transform the points  $x = \pm 0.7745966692, 0$  to

the interval  $[0, \pi]$ . We have the transformed points as

$$0 + \frac{\pi}{2} (\pm 0.7745966692 + 1) \Rightarrow q_1 = 0.354063, \quad q_3 = 2.78753$$

and for the quadrature point  $x = 0$  we have

$$0 + \frac{\pi}{2} (0 + 1) \Rightarrow q_2 = \frac{\pi}{2} = 1.570796$$

The weights are

$$w_1 = w_3 = \frac{\pi}{2} (0.5555555) \quad w_2 = \frac{\pi}{2} (0.8888888)$$

Using these points and weights gives the approximation

$$\begin{aligned} \int_0^{\pi} \sin x \, dx &\approx \frac{\pi}{2} \left[ 0.5555555 \sin(0.354063) + 0.8888888 \sin\left(\frac{\pi}{2}\right) \right. \\ &\quad \left. + 0.5555555 \sin(2.78753) \right] = 2.00136 \end{aligned}$$

giving an error of 0.001362.

Note that the interval is quite large (length  $\pi$ ) and we are only using two or three quadrature points so our accuracy is quite good. If we use Simpson's Rule to

approximate this integral we get

$$\frac{\pi}{6} \left( \sin(0) + 4 \sin\left(\frac{\pi}{2}\right) + \sin(\pi) \right) = 2.0944$$

with an error of 0.094395. So performing both Simpson's Rule and the 3-point Gauss Rule require three function evaluations but the error in the Gauss Rule is almost seventy times smaller.

### Summary for Gauss quadrature

- We use  $N$  quadrature points.
- The quadrature points are symmetric on  $[-1, 1]$ .
- The degree of precision of the rule is  $2N - 1$ , i.e., it integrates polynomials of degree  $2N - 1$  or less exactly.
- The rule can be applied on any interval using an appropriate transformation.
- The rules can easily be used as composite rules just like Newton-Cotes rules.
- Gauss rules are preferred over Newton-Cotes rules because the accuracy is greater for the same number of function evaluations.

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## Gauss Rules other than Gauss-Legendre

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As we saw, the quadrature points for Gauss-Legendre rules are the roots of the Legendre polynomials. However, we can also derive Gauss rules using other orthogonal polynomials.

### Gauss-Laguerre Quadrature Rules

Consider integrals which have a semi-infinite domain of the form

$$\int_0^{\infty} e^{-x} f(x) dx$$

In this case we use quadrature points which are roots of the Laguerre polynomial  $L_n$ . Like Legendre polynomials, Laguerre polynomials can be obtained from a recursion formula and the first three are given here

$$L_1 = 1 - x, \quad L_2 = \frac{1}{2}(x^2 - 4x + 2), \quad L_3 = \frac{1}{6}(-x^3 + 9x^2 - 18x + 6)$$

Once we have the roots for the quadrature points, then we determine the weights

by fitting the Lagrange interpolating polynomial. For example, for the one-point Gauss-Laguerre formula we have the quadrature point  $q_1 = 1$  so we can simply use  $p_0(x) = 1$ . Since we want a one point formula of the form

$$\int_0^{\infty} e^{-x} f(x) dx \approx f(1)w_1$$

we take the Lagrange polynomial and integrate

$$\int_0^{\infty} e^{-x} f(1)\mathcal{L}_1(x) dx = f(1) \int_0^{\infty} e^{-x}(1) dx = f(1) \cdot 1$$

so  $w_1 = 1$ .

One can also obtain an explicit formula for the weights in terms of the Laguerre polynomial evaluated at the quadrature point.

What do we do if we have an integral with a semi-infinite domain but there is no  $e^{-x}$  in the integrand? We simply do a change of variables as the following example illustrates.

**Example** Approximate the integral

$$\int_0^{\infty} \ln(1 + e^{-x}) dx = \frac{\pi^2}{12} = 0.822467$$

using a 2-point Gauss Legendre rule.

We must first rewrite the integral so that it is in a form we can use. To this end, we have

$$\int_0^{\infty} \ln(1 + e^{-x}) dx = \int_0^{\infty} e^{-x} e^x \ln(1 + e^{-x}) dx = \int_0^{\infty} e^{-x} f(x) dx$$

where  $f(x) = e^x \ln(1 + e^{-x})$ . The quadrature points are  $q_1 = 0.585786437627$ ,  $q_2 = 3.41421356237$  and the weights are  $w_1 = 0.853553390593$  and  $w_2 = 0.146446609407$ . Applying the rule gives

$$\begin{aligned} \int_0^{\infty} \ln(1+e^{-x}) dx &\approx 0.853553390593e^{q_1} \ln(1+e^{-q_1}) + 0.146446609407e^{q_2} \ln(1+e^{-q_2}) \\ &= 0.822659 \end{aligned}$$

## Gauss-Hermite Quadrature Rules

In Gauss-Hermite we consider integrals of the form

$$\int_{-\infty}^{\infty} e^{-x^2} f(x) dx$$

Here the quadrature points are the roots of the Hermite polynomials and the weights are determined as before. These are used when we have an integral with both limits of integration being infinite.

So for every orthogonal polynomial we can generate a family of Gauss rules.

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## Improper Integrals

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A **proper integral** is a definite integral whose integrand is continuous over the bounded domain of integration; any other integral is called an **improper integral**. For example,  $\int_0^{\infty} \ln(1 + e^{-x}) dx$  we considered is an improper integral because we are not integrating over a bounded domain. Other integrals may have discontinuities in their integrands and are thus improper.

We have seen that if we have one or both of our limits of integration as infinity then we can use Gauss-Laguerre or Gauss-Hermite quadrature rules. Often, we can also handle this situation by other techniques which we demonstrate here.

### Integrals over unbounded domains

If one or both of our limits of integration are infinite then there are several approaches we can try.



- Use a special quadrature rule such as Gauss-Laguerre or Gauss-Hermite (depending on whether we have one or both limits as infinite)
- Truncate the interval to a finite one
- Perform a change of variables to transform the integral to one over a finite domain.

If the integrand decays fast enough, then we can truncate the domain as illustrated in the next example.

**Example** Approximate  $\int_0^{\infty} \ln(1 + e^{-x}) dx$  by truncating the domain. If we plot the integrand we see that it decays very rapidly to zero. From the graph we choose to truncate the domain at  $x = 6$  so all we have to do is evaluate  $\int_0^6 \ln(1 + e^{-x}) dx$  using any of the techniques we have learned.

Another approach is to transform the integral so that it no longer is over an infinite domain. Care must be used here or else the integrand may oscillate and cause problems.

**Example** Approximate  $\int_0^{\infty} \ln(1 + e^{-x}) dx$  by performing a change of variables

so that the domain is finite. We want to define a new variable  $t$  such that when  $x = \infty$  then  $t$  is bounded. If we let  $x = \frac{1}{t} - 1$  then when  $x = 0$  then  $t = 1$  and when  $x = \infty$ ,  $t = 0$ . This gives

$$x = \frac{1}{t} - 1 \Rightarrow dx = -\frac{1}{t^2} dt$$

so that

$$\int_0^{\infty} \ln(1 + e^{-x}) dx = - \int_1^0 \ln(1 + e^{1-1/t}) \frac{1}{t^2} dt = \int_0^1 \ln(1 + e^{1-1/t}) \frac{1}{t^2} dt$$

## Integrals with Singularities

Suppose we want to approximate an integral such as

$$\int_0^1 \frac{e^{-x}}{x^{2/3}} dx$$

If we tried to apply a formula such as Simpson's Rule, then we are in trouble because the integrand becomes infinite as  $x \rightarrow 0$ . However, if we use a rule such as an open Newton-Cotes formula or Gauss quadrature rule which does not use the endpoints then we can typically get a good answer.

What if the singularity doesn't occur at the endpoints of the interval? If we have an integral such as

$$\int_0^2 \frac{1}{x-1} dx$$

where the integrand is not defined at  $x = a$  then we break it into two integrals

$$\int_0^2 \frac{1}{x-1} dx = \int_0^1 \frac{1}{x-1} dx + \int_1^2 \frac{1}{x-1} dx$$

and use a rule on each integral which does not use the endpoints as quadrature points.

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## Integration Using the Monte Carlo Method

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**Monte Carlo** methods are a widely used class of computational algorithms. In its simplest form, the Monte Carlo algorithm can be used for straightforward computations such as approximating a scalar, an area or volume. More complicated variants of the algorithm can be used in areas such as computational physics, chemistry, applied mathematics, for example. We will return to look at Monte Carlo methods in more detail towards the end of the semester.

Monte Carlo methods were originally called **statistical sampling** methods due to the use of **randomness**.

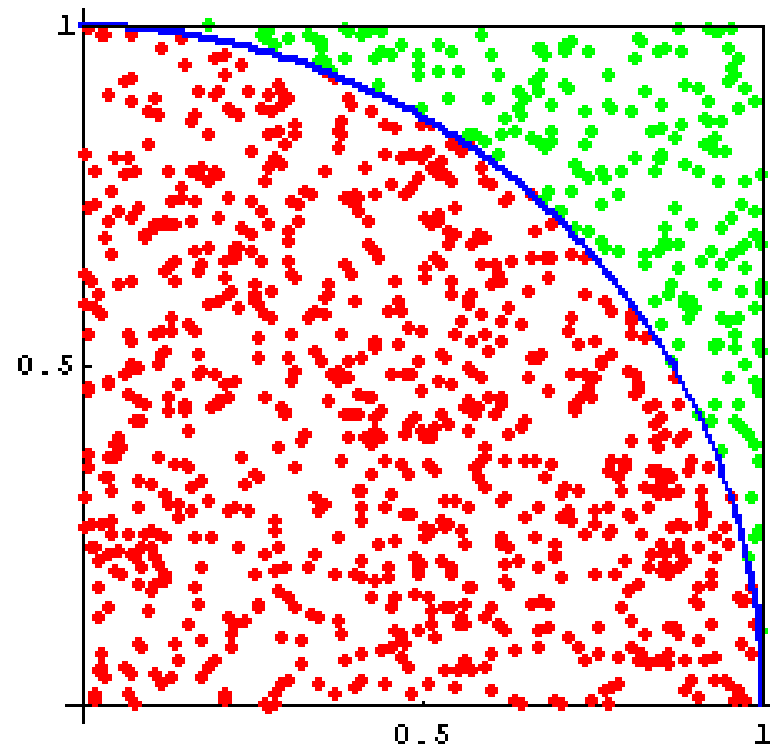
Historically these methods were developed by John von Neumann, Enrico Fermi, Stanislaw Ulam and Nicholas Metropolis.

To describe the Monte Carlo method in its simplest form consider the problem of approximating  $\pi$ .

- We know that the area of the *unit* circle (with radius 1) is just  $\pi$ . So the area of the portion of the unit circle in the first quadrant is just  $\pi/4$ .
- We choose random numbers  $x, y$  where  $0 \leq x \leq 1, 0 \leq y \leq 1$ .
- If the point  $(x, y)$  lies in or on the circle (i.e.,  $x^2 + y^2 \leq 1$ ) then we record this as a “hit”.
- The area of the circle ( $\pi$ ) is then approximated by

$$4 \times \frac{\text{points satisfying } x^2 + y^2 \leq 1}{N}$$

where  $N$  is the total number of random points  $(x, y)$  that we generate.



Now we want to apply this technique to approximate an integral.

- Suppose we want to evaluate  $\int_a^b f(x) dx$
- If  $f(x) \geq 0$  for  $a \leq x \leq b$  then we know that this integral represents the area under the curve  $y = f(x)$  and above the  $x$ -axis.

- So far we have looked at standard **deterministic** numerical integration rules approximate this integral by

$$\sum_{i=1}^N w_i f(q_i)$$

- The Monte Carlo method is a **probabilistic** approach to approximating the integral.
- We determine a simple region  $a_1 \leq x \leq a_2, b_1 \leq y \leq b_2$  which contains  $f(x)$  for  $a \leq x \leq b$ . Then we generate a random number  $(\hat{x}, \hat{y})$  where  $a_1 \leq \hat{x} \leq a_2, b_1 \leq \hat{y} \leq b_2$ . We then determine if  $(\hat{x}, \hat{y})$  lies on or below the graph of  $f(x)$ , i.e., in the desired area. If so, it is labeled a "hit" and we increase our counters appropriately. We continue this process.



To approximate the integral using Monte Carlo we

- choose a simpler region (such as a rectangle) which includes the area you want to determine
- generate a random point in the simpler region
- determine if random point is in desired region
- take area as fraction of area of simpler region

**Example** Approximate

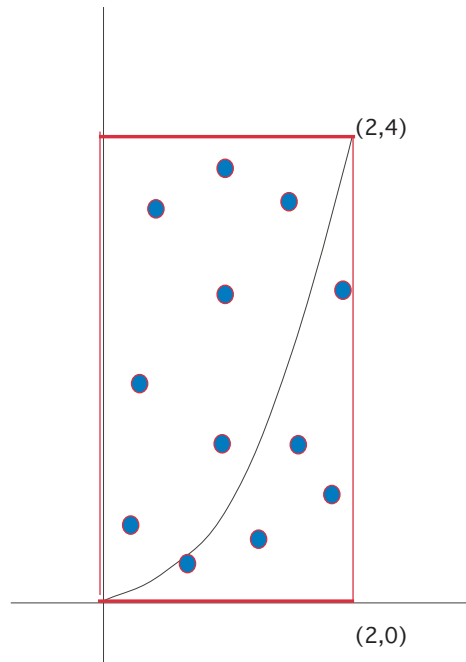
$$\int_0^2 x^2 dx$$

using the Monte Carlo method.

Here we know that  $0 \leq x^2 \leq 4$  on the domain so we take the square with base two and height four as our bounding region. We generate a random point  $(x, y)$  where  $0 \leq x \leq 2$ ,  $0 \leq y \leq 4$  and then check to see if it lies below the curve or above the curve. To do this, we simply evaluate the integrand at the random  $x$  value and if  $y \leq f(x)$  then we call it a "hit" otherwise, not. We continue in this manner. Our approximation to the integral is simply the usual fraction of the area of the testing region. Here the area of the testing region is 8 so we have

$$\frac{\text{number of hits}}{\text{number of points}} \times 8$$

Of course we could have chosen a different testing region.



12 random points generated and  
5 in the desired region

**Example** Approximate  $\int_0^\pi \cos(4 \sin(x)) dx$  using Monte Carlo. We don't see the kind of rapid convergence we are used to! (Table from J. Burkardt)

N	MC error	NC error
1	0.598	0.805
2	1.892	4.389
3	1.208	0.925
4	1.312	0.201
5	1.316	0.662
6	0.618	0.348
7	0.195	0.025
8	0.552	0.372
9	0.157	0.065
10	1.061	0.036
11	0.117	0.014
12	0.517	0.010
13	0.591	0.003
14	0.222	0.001
15	0.034	0.002
16	0.584	0.001
17	0.065	2e-4
18	0.526	1e-4
19	0.466	9e-5
20	0.532	5e-5

As you can see from the results, it takes a lot of random points to get several digits of accuracy for MC and the error is not monotonically decreasing. In one dimension, deterministic quadrature rules are usually preferable to Monte Carlo but in higher dimensions, Monte Carlo often is better.

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## Integration in Higher Dimensions

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So far we have only looked at integrals in one dimension so the domain of integration is always an interval. Oftentimes we have to compute integrals in two, three, and higher dimensions. If the domain is the tensor product of intervals then we can extend our one-dimensional Newton-Cotes and Gauss rules easily. However, if the dimension is high, then these may not be feasible. For example, if we have extend a rule in one dimension which uses two points then in nine dimensions it uses  $2^9 = 512$  quadrature points and in twenty dimensions we have  $10^6$  points!

For integrals where the domain of integration is complicated, we can not easily extend our one-dimensional rules so we have to decide how these integrals can be approximated.

Integrals whose domain is a tensor product  $[a_i, b_i]^n$

For simplicity suppose we have the integral

$$\int_{a_1}^{b_1} \int_{a_2}^{b_2} f(x, y) dy dx$$

that we want to approximate using a Gauss-Legendre quadrature rule. The domain of integration is the rectangle  $[a_1, b_1] \times [a_2, b_2]$ .

In one dimension we employed the Gauss-Legendre quadrature rules on  $[-1, 1]$ . If we take the tensor products of a  $p$ -point Gauss rule in each direction in  $\mathbb{R}^2$  then we would have one point for the tensor product of the one-point rule, four points for the tensor product of the two-point rule, etc. The quadrature points in two dimensions formed by the tensor product of one-point through three-point Gauss quadrature rules are described below. Note that in three dimensions we have 1, 8, and 27 quadrature points for tensor products of these three quadrature rules.

To apply these rules to an integral over an arbitrary rectangular domain, we must perform a change of variables in both the  $x$  and  $y$  directions analogous to the




	1-D rule	# points in $\mathbb{R}^2$	points $q_i$ & weights $w_i$
	1 point Gauss	1	$q_1 = (0, 0) \quad w_1 = 4$
	2 point Gauss	4	$q_i = \frac{1}{\sqrt{3}} \{(-1, -1), (1, -1), (-1, 1), (1, 1)\}$ $w_i = 1$
	3 point Gauss	9	$q_i = \sqrt{\frac{3}{5}} \{(-1, -1), (0, -1), (1, -1), (-1, 0),$ $((0, 0), (1, 0), (-1, 1), (0, 1), (1, 1))\}$ $w_i = \frac{1}{81} \{25, 40, 25, 40, 64, 40, 25, 40, 25\}$

TABLE 0.2

*Tensor product of Gauss quadrature rules in two dimensions*

one-dimensional case.

The Newton-Cotes formulas can be extended to domains defined by  $[a_i, b_i]^n$  in the same manner.

Extending the deterministic quadrature rules in one dimension works well on a



rectangular domain in two or three dimensions. However, if we have a high dimensional domain even if it is a tensor product of 1-D intervals can be prohibitively time consuming.

Consider a 10-D integral (far less uncommon than you would think) with simple boundaries

$$I = \int_0^1 \int_0^1 \cdots \int_0^1 f(x_1, x_2, \dots, x_{10}) dx_{10} \dots dx_2 dx_1.$$

Even if you considered 10 points along each dimension  $x_i$ , you would have to  $10^{10}$  points to evaluate the function at. If your integrand required a millisecond to compute, then evaluating simply the function at all the grid-points would require more than 100 days. So this is not feasible.

What can be done instead? A common approach is to use Monte Carlo. We saw that in one dimension Monte Carlo required a lot of points to get an accurate solution and really had no advantage over deterministic methods except maybe for its simplicity. In higher dimensions it is actually more feasible than most standard deterministic rules.

The reason for this is that the error in Monte Carlo vanishes like

$$\frac{1}{\sqrt{N}}$$

where  $N$  is the number of points. In 1-D most of the methods we considered are better than this.

However, the error in Monte Carlo does not depend on the spatial dimension. This is in contrast to deterministic methods; for example, the error in Simpson's rule which vanishes like

$$\frac{1}{N^{4/d}}$$

where  $d$  is the spatial dimension.