

Numerical Integration

1 Quadrature Rules

- formulas for numerical integration
- deriving quadrature rules

2 Composite Quadrature Rules

- the composite trapezoidal rule
- a Julia function

3 Newton-Cotes Formulas

- integrate the interpolating polynomial

MCS 471 Lecture 25

Numerical Analysis

Jan Verschelde, 19 October 2022

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quadrature rules

Given a function $f(x)$ over an interval $[a, b]$, our problem is to approximate the definite integral of f over $[a, b]$, by a weighted sum of function values:

$$\int_a^b f(x) dx \approx w_1 f(x_1) + w_2 f(x_2) + \cdots + w_n f(x_n).$$

The *quadrature rule* is defined by

- interpolation points $x_i \in [a, b]$, $x_1 < x_2 < \cdots < x_n$; and
- weights w_i to multiply the function values with.

the midpoint and trapezoidal rule

The midpoint rule is defined by

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

The area under $y = f(x)$ is approximated

by the area of the rectangle with base $b - a$ and height $f\left(\frac{a + b}{2}\right)$.

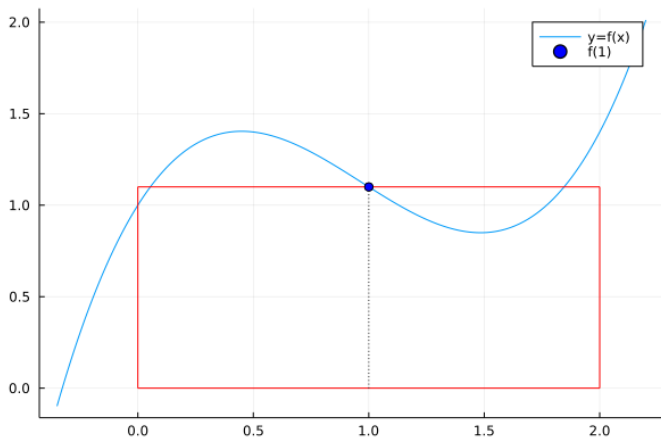
The trapezoidal rule is defined by

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

The area under $y = f(x)$ is approximated

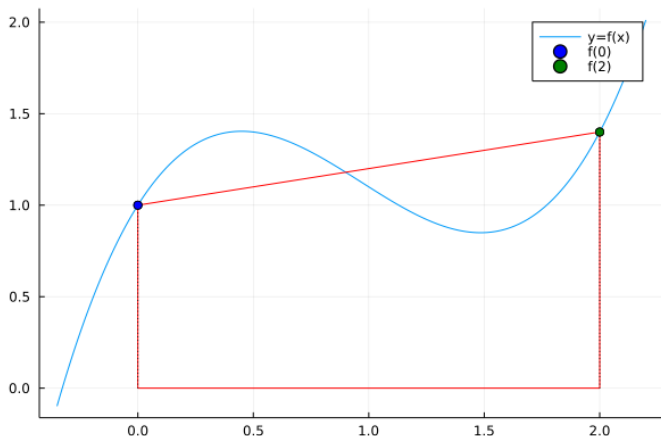
by the area of the trapezoid with base $b - a$ and heights $f(a)$ and $f(b)$.

the midpoint rule



$\int_0^2 f(x) dx$, the area under the blue curve, for $x \in [0, 2]$,
is approximated by $2 f(1)$, the area of the red rectangle.

the trapezoidal rule



$\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0, 2]$,
is approximated by $\frac{2-0}{2} (f(2) - f(0))$, the area of the red trapezoid.

error terms

For the polynomial p interpolating f at points x_0, x_1, \dots, x_n , we have

$$p(x) = f(x) + \frac{f^{n+1}(\alpha)}{(n+1)!} (x - x_0)(x - x_1) \cdots (x - x_n),$$

for some $\alpha \in [a, b]$.

Then we can derive the following error formula:

$$\int_a^b f(x) dx = \int_a^b p(x) dx - \frac{f^{n+1}(\alpha)}{(n+1)!} \int_a^b (x - x_0)(x - x_1) \cdots (x - x_n) dx.$$

So we have the error is

$$\left| \frac{f^{n+1}(\alpha)}{(n+1)!} \int_a^b (x - x_0)(x - x_1) \cdots (x - x_n) dx \right|.$$

the error of the trapezoidal rule

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

We have $x_0 = a$ and $x_1 = b$ in the error formula:

$$\left| \frac{f^{n+1}(\alpha)}{(n+1)!} \int_a^b (x-x_0)(x-x_1) \cdots (x-x_n) dx \right|.$$

We compute:

$$\int_a^b (x-a)(x-b) dx = \frac{(b-a)^3}{6}.$$

So the error for the trapezoidal rule is $\left| \frac{f''(\alpha)}{12} \right| (b-a)^3$.

Exercise 1:

Compute the error formula for the midpoint rule.

degree of precision

The cost of a quadrature rule is determined by the number of function values, or equivalently, the number of interpolation points.

Definition

A quadrature rule has *degree of precision* d if the rule integrates all polynomials of degree d or less exactly.

Because \int_a^b is a linear operator:

$$\int_a^b c_d x^d + \cdots + c_1 x + c_0 dx = \int_a^b c_d x^d dx + \cdots + \int_a^b c_1 x dx + \int_a^b c_0 dx,$$

it suffices to compute the degree of precision for the basis functions.

the degree of precision of the midpoint rule

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

$$f = 1 : \int_a^b 1 dx = b - a, \quad R(1) = b - a$$

$$f = x : \int_a^b x dx = \frac{b^2}{2} - \frac{a^2}{2}, \quad R(x) = (b-a)(a+b)/2$$

$$f = x^2 : \int_a^b x^2 dx = \frac{b^3}{3} - \frac{a^3}{3}, \quad R(x^2) = (b-a)((a+b)/2)^2$$

We see that $R(1)$ and $R(x)$ are exact, but $R(x^2) \neq \int_a^b x^2 dx$.

Exercise 2:

Compute the degree of precision of the trapezoidal rule.

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- **deriving quadrature rules**

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deriving a quadrature rule

Determine the weights w_0 , w_1 and w_2 in

$$\int_a^b f(x) dx \approx w_0 f(a) + w_1 f\left(\frac{a+b}{2}\right) + w_2 f(b),$$

so the degree of precision is as high as possible.

$$f = 1 : \int_a^b 1 dx = b - a = w_0 + w_1 + w_2$$

$$f = x : \int_a^b x dx = \frac{b^2}{2} - \frac{a^2}{2} = w_0 a + w_1 \left(\frac{a+b}{2}\right) + w_2 b$$

$$f = x^2 : \int_a^b x^2 dx = \frac{b^3}{3} - \frac{a^3}{3} = w_0 a^2 + w_1 \left(\frac{a+b}{2}\right)^2 + w_2 b^2$$

solving a linear system

$$\int_a^b 1 dx = b - a = w_0 + w_1 + w_2$$
$$\int_a^b x dx = \frac{b^2}{2} - \frac{a^2}{2} = w_0 a + w_1 \left(\frac{a+b}{2} \right) + w_2 b$$
$$\int_a^b x^2 dx = \frac{b^3}{3} - \frac{a^3}{3} = w_0 a^2 + w_1 \left(\frac{a+b}{2} \right)^2 + w_2 b^2$$

In matrix format:

$$\begin{bmatrix} 1 & 1 & 1 \\ a & (a+b)/2 & b \\ a^2 & ((a+b)/2)^2 & b^2 \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} b-a \\ b^2/2 - a^2/2 \\ b^3/3 - a^3/3 \end{bmatrix}$$

Observe the structure: we have a Vandermonde matrix (transposed).

solving with SymPy gives Simpson's rule

```
julia> using SymPy
julia> a,b,w0,w1,w2 = Sym("a,b,w0,w1,w2");
julia> eq1 = w0 + w1 + w2;
julia> eq2 = a*w0 + (a+b)*w1/2 + b*w2;
julia> eq3 = a^2*w0 + (a+b)^2*w1/4 + b^2*w2;
julia> solve([eq1 - b+a,
              eq2 - b^2/2 + a^2/2,
              eq3 - b^3/3 + a^3/3], [w0,w1,w2])
```

Dict{Any,Any} with 3 entries:

$$w2 \Rightarrow -a/6 + b/6$$

$$w0 \Rightarrow -a/6 + b/6$$

$$w1 \Rightarrow -2*a/3 + 2*b/3$$

$$\int_a^b f(x)dx \approx \left(\frac{b-a}{6}\right) f(a) + 2\left(\frac{b-a}{3}\right) f\left(\frac{a+b}{2}\right) + \left(\frac{b-a}{6}\right) f(b)$$

making another quadrature rule

Exercise 3:

Consider the quadrature rule

$$\int_{-a}^a f(x) dx \approx w_1 f\left(\frac{-a}{2}\right) + w_2 f\left(\frac{a}{2}\right), \quad \text{for } a > 0.$$

- 1 Determine the weights w_1 and w_2 to obtain the highest possible degree of precision.
- 2 What is the degree of precision of your rule?
Verify for 1 , x , and also x^2 .

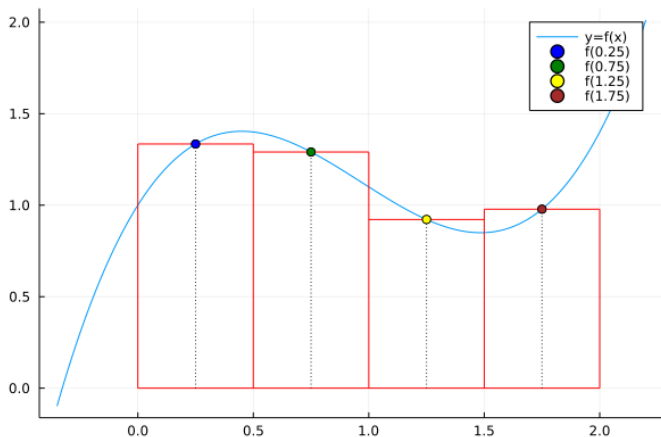
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the composite midpoint rule



$\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0, 2]$,
is approximated by the sum of the areas of four red rectangles.

composite quadrature rules

A composite quadrature rule over $[a, b]$ consists in

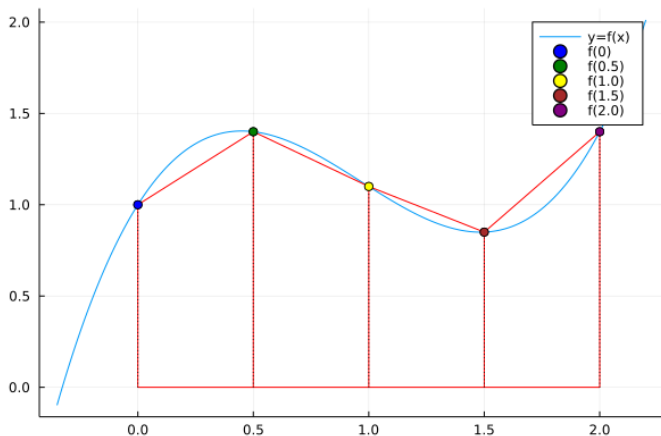
- 1 dividing $[a, b]$ in n subintervals, $h = (b - a)/n$;
- 2 applying a quadrature rule to each subinterval $[a_i, b_i]$, with $a_i = a + (i - 1)h$, and $b_i = a + ih$, for $i = 1, 2, \dots, n$;
- 3 summing up the approximations on each subinterval.

Example: $[a, b] = [0, 1]$, $n = 4$: $h = 1/4$, and the subintervals are $[0, 1/4]$, $[1/4, 1/2]$, $[1/2, 3/4]$, $[3/4, 1]$.

Exercise 4:

Derive the formula for the composite midpoint rule over n subintervals to approximate the integral of $f(x)$ over $[a, b]$.

the composite trapezoidal rule



$\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0, 2]$,
is approximated by the sum of the areas of four red trapezoids.

the composite trapezoidal rule

For $n = 1$:

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

For $n > 1$, $h = (b-a)/n$, $a_i = a + (i-1)h$, $b_i = a + ih$:

$$\begin{aligned} \int_a^b f(x) dx &= \sum_{i=1}^n \int_{a_i}^{b_i} f(x) dx \\ &= \sum_{i=1}^n \frac{h}{2} (f(a_i) + f(b_i)) \\ &= \frac{h}{2} (f(a) + f(b)) + h \sum_{i=1}^{n-1} f(a + ih) \end{aligned}$$

Observe that $a_i = b_{i-1}$ and the value $f(b_{i-1})$ at the right of the $(i-1)$ -th interval equals the value $f(a_i)$ at the left of the i -th interval.

the error of the composite trapezoidal rule

The error of the trapezoidal rule for f over $[a, b]$ is

$$\left| \frac{f''(\alpha)}{12} \right| (b-a)^3,$$

for some $\alpha \in [a, b]$. For the composite rule over n subintervals, the length of each subinterval is $h = (b-a)/n$.

The error of the composite trapezoidal rule is then

$$\sum_{i=1}^n \left| \frac{f''(\alpha_i)}{12} \right| h^3,$$

for $\alpha_j \in [a_j, b_j]$. If we apply the mean value theorem on f'' , then there exists an $\alpha \in [a, b]$ such that $nf''(\alpha)$ is the sum over all $f''(\alpha_j)$'s.

The error is then $\left| \frac{nf''(\alpha)}{12} \right| h^3 = \left(\frac{b-a}{12} \right) |f''(\alpha)| h^2$, which is $O(h^2)$.

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a Julia function

```
"""
```

Applies the composite trapezoidal rule to approximate the integral of the function f over the interval $[a,b]$, using n subintervals.

```
Example: t = comptrap(cos,0,pi/2,100)
```

```
"""
```

```
function comptrap(f::Function,a::Float64,  
                  b::Float64,n::Int64)
```

```
    h = (b-a)/n
```

```
    t = (f(a) + f(b))/2
```

```
    for i = 1:n-1
```

```
        t = t + f(a+i*h)
```

```
    end
```

```
    t = t*h
```

```
    return t
```

```
end
```

testing the `comptrap` function

```
"""  
Applies the composite trapezoidal rule  
to the area under the unit circle.  
"""  
  
function main()  
    f(x) = sqrt(1 - x^2)  
    exact = pi/4  
    N = 1  
    for i=1:21  
        t = comptrap(f,0.0,1.0,N)  
        strnbr = @sprintf("%7d", N)  
        strval = @sprintf("%.16e", t)  
        strerr = @sprintf("%.2e", abs(t-exact))  
        println(" $strnbr  $strval  $strerr")  
        N = 2*N  
    end  
end
```

running the program

1	5.0000000000000000e-01	2.85e-01
2	6.8301270189221930e-01	1.02e-01
4	7.4892726702561019e-01	3.65e-02
8	7.7245478608929330e-01	1.29e-02
16	7.8081325945693536e-01	4.58e-03
32	7.8377560571928273e-01	1.62e-03
64	7.8482422819492148e-01	5.74e-04
128	7.8519519809915361e-01	2.03e-04
256	7.8532639573930751e-01	7.18e-05
512	7.8537278817991363e-01	2.54e-05
1024	7.8538919163475496e-01	8.97e-06
2048	7.8539499135286062e-01	3.17e-06
4096	7.8539704190193971e-01	1.12e-06
8192	7.8539776688742258e-01	3.97e-07
16384	7.8539802320972329e-01	1.40e-07
32768	7.8539811383356084e-01	4.96e-08
65536	7.8539814587395984e-01	1.75e-08
131072	7.8539815720195694e-01	6.20e-09
262144	7.8539816120701722e-01	2.19e-09
524288	7.8539816262302165e-01	7.74e-10
1048576	7.8539816312366018e-01	2.74e-10

cost and convergence

Doubling the number of function evaluations,

524288	7.8539816262302165e-01	7.74e-10
1048576	7.8539816312366018e-01	2.74e-10

from 524,288 to 1,048,576, the error decreases from 7.7×10^{-10} to 2.7×10^{-10} , a reduction factor of 2.85.

The convergence is linear, and too slow.

Exercise 5:

Apply the composite midpoint rule to $\int_0^1 \sqrt{1-x^2} dx$
for a number of intervals ranging from 1 to 2^{20} .

Describe the convergence? Compare with the application of the composite trapezoidal rule to this problem.

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Newton-Cotes Formulas

To approximate $\int_a^b f(x)dx$, with $n + 1$ function evaluations:

- 1 Let $h = (b - a)/n$ and set $x_i = a + ih$, for $i = 0, 1, \dots, n$.
- 2 Let p be the polynomial interpolating at $(x_i, f(x_i))$: $p(x_i) = f(x_i)$.
- 3 Then the rule is

$$\int_a^b p(x)dx \quad \text{with error term} \quad E = \left| \int_a^b \prod_{i=0}^n (x - x_i) dx \right|.$$

Such rules are called *Newton-Cotes formulas*.

We have seen two examples:

- 1 $n = 1$: the trapezoidal rule,
- 2 $n = 2$: Simpson's rule.

recall Lagrange interpolation

Given (x_i, f_i) , for $i = 0, 1, \dots, n$, and for any $j \neq i$: $x_j \neq x_i$, the Lagrange form of the interpolating polynomial p is

$$p(x) = f_0 l_0(x) + f_1 l_1(x) + \dots + f_n l_n(x), \quad l_j(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \left(\frac{x - x_j}{x_i - x_j} \right).$$

Then the quadrature rule is

$$\int_a^b p(x) dx = f_0 \underbrace{\int_a^b l_0(x) dx}_{w_0} + f_1 \underbrace{\int_a^b l_1(x) dx}_{w_1} + \dots + f_n \underbrace{\int_a^b l_n(x) dx}_{w_n}.$$

The weights of the Newton-Cotes formulas are the integrals of the Lagrange polynomials.