Romberg Integration

1. Adaptive Integration
   - stopping the composite trapezoidal rule
   - a Julia function
2. The Euler-Maclaurin Summation Formula
   - justifying the use of extrapolation
   - a Julia function
3. Approximating π
   - applying the composite trapezoidal rule

MCS 471 Lecture 26
Numerical Analysis
Jan Verschelde, 21 October 2022

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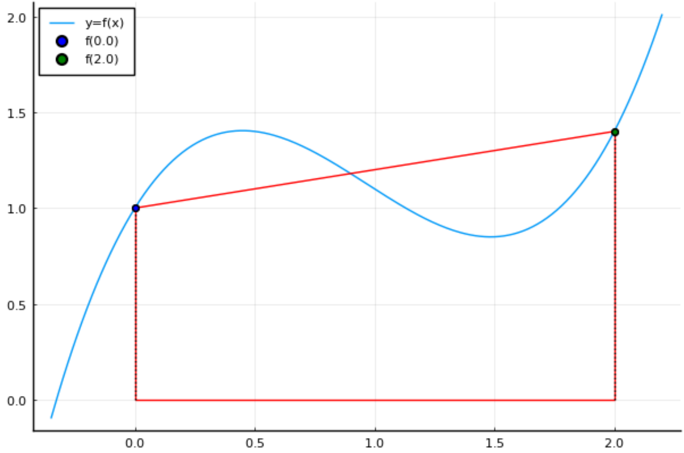
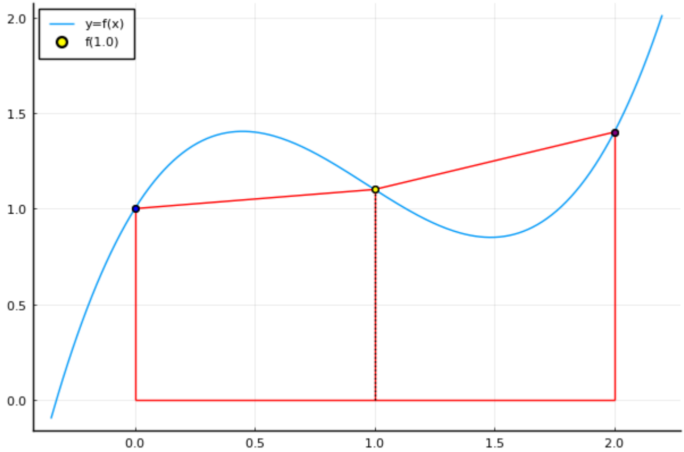
the trapezoidal rule starts with 2 function evaluations



$\displaystyle\int_0^2 f(x)dx$, 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.

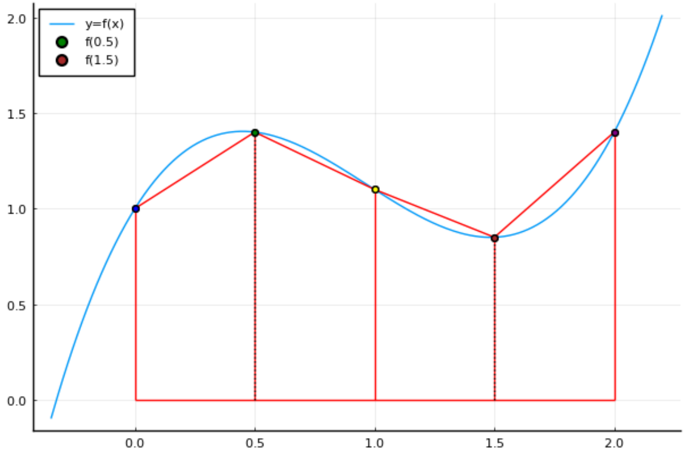
one extra function evaluation



$\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0, 2]$,

is approximated by the sum of the areas of two red trapezoids.

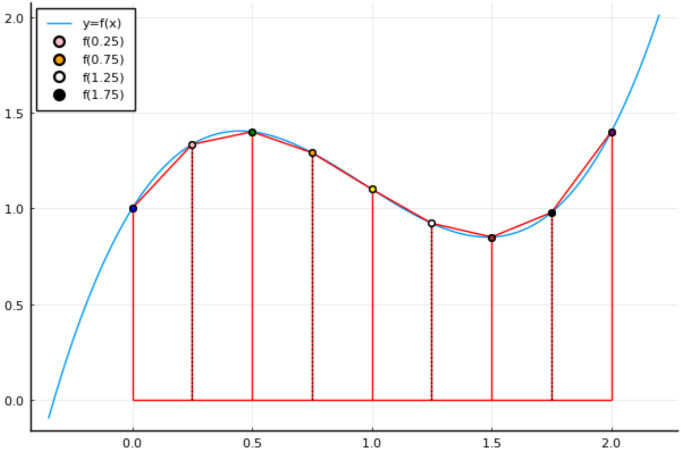
two extra function evaluations



$$\int_0^2 f(x)dx, \text{ the area under the blue curve, for } x \in [0, 2],$$

is approximated by the sum of the areas of four red trapezoids.

four extra function evaluations



$\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0, 2]$,

is approximated by the sum of the areas of eight red trapezoids.

stopping the composite trapezoidal rule

The composite trapezoidal rule
applied to $f(x)$ over $[a, b]$ with n subintervals is

$$\int_a^b f(x)dx \approx \frac{h}{2}\Big(f(a) + f(b)\Big) + h\sum_{i=1}^{n-1} f(a+ih), \quad h = \frac{b-a}{n}.$$

The composite trapezoidal rule is straightforward to apply,
but in general we do not know a good apriori value for n.

Our problem is to apply the composite trapezoidal rule in an iterative algorithm: we stop when the accuracy of the approximation is good.

We can estimate the accuracy by comparing
the last two approximations.

an iterative composite trapezoidal rule

Input: $f(x)$ and $[a,b]$ define $\displaystyle\int_a^b f(x)dx$,

N is an upper bound on the number of subintervals,

ϵ is the accuracy requirement.

Output: an approximation for $\displaystyle\int_a^b f(x)dx$

n is the number of subintervals computed.

$$T_1 := \frac{b-a}{2}\Big(f(a)+f(b)\Big)$$

for n from 2 to N do

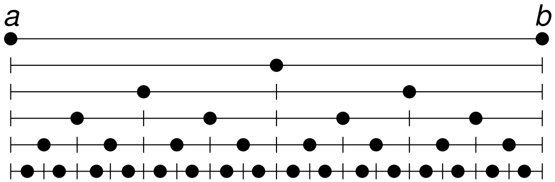
$h := (b-a)/n$

$$T_n := \frac{h}{2}\Big(f(a)+f(b)\Big) + h\sum_{i=1}^{n-1} f(a+ih)$$

if $|T_n - T_{n-1}| < \epsilon$ then return (T_n, n)

return (T_N, N)

the new function evaluations



The number of new function evaluations is $1, 2, 4, 8, 16$.

Observe the distance between the new function evaluations.

the formulas

$$T_n = \frac{b-a}{2n}\left(f(a)+f(b)\right) + \frac{b-a}{n}\sum_{i=1}^{n-1} f\left(a + i\frac{b-a}{n}\right)$$

$$T_{2n} = \frac{b-a}{4n}\left(f(a)+f(b)\right) + \frac{b-a}{2n}\sum_{i=1}^{2n-1} f\left(a + i\frac{b-a}{2n}\right)$$

We can separate the new function evaluations for the previous sum:

$$T_{2n} = \frac{1}{2}T_n + \frac{b-a}{2n}\sum_{i=1}^{n-1} f\left(a + \frac{b-a}{2n} + i\frac{b-a}{n}\right)$$

on the composite midpoint rule

Exercise 1:

Consider the midpoint rule: $\int_a^b f(x)dx = (b-a)f\left(\frac{a+b}{2}\right)$.

1. Give the formula to apply the composite midpoint rule on n subintervals of $[a,b]$.
2. In order to recycle all function evaluations in the next step in an iterative application of the composite midpoint rule, justify why each subinterval should be divided in three.

Exercise 2:

Write a Julia function to apply the composite midpoint rule to

$\int_0^{\pi/2} \cos(x)dx$ with 10^{-4} as the tolerance for the stopping criterion.

Compare the results with the adaptive composite trapezoidal rule.

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specifications of a Julia function

```
"""
Returns a vector of at most n approximations
for the definite integral of the function f
over the interval [a,b], the i-th entry in the
returned vector uses 2^i function evaluations.
Stops when the difference between two
consecutive approximations is less than tol.

Example:

    t = adaptrap(cos,0,pi/2,10,1.e-5)
"""
function adaptrap(f::Function,
                  a::Float64,b::Float64,
                  n::Int64,tol::Float64)
```

definition of the function

```
    t = zeros(n)
    h = (b-a)           # size of subinterval
    m = 1               # number of subintervals
    t[1] = (f(a) + f(b))*h/2
    for i = 2:n
        h = h/2
        for j=0:m-1
            t[i] = t[i] + f(a+h+j*2*h)
        end;
        t[i] = t[i-1]/2 + h*t[i]
        if(abs(t[i] - t[i-1])) < tol
            return t[1:i], i
        end
        m = 2*m
    end
    return t, n
end
```

the main test function

```
"""
Applies adaptive integration.
"""
function main()
    exact = 1.0
    n = 20
    tol = 1.0e-4
    t, nit = adaptrap(cos,0.0,pi/2,n,tol)
    println("The composite trapezoidal rule :")
    for i=1:length(t)
        strerr = @sprintf("%.2e", abs(exact - t[i]))
        strapp = @sprintf("%.16e", t[i])
        println("$strapp  $strerr")
    end
    print("The number of iterations : ")
    println(nit)
end
```

running the script

The stop tolerance is `1.0e-4`.

```
The composite trapezoidal rule :
7.8539816339744828e-01  2.15e-01
9.4805944896851990e-01  5.19e-02
9.8711580097277540e-01  1.29e-02
9.9678517188616966e-01  3.21e-03
9.9919668048507226e-01  8.03e-04
9.9979919432001874e-01  2.01e-04
9.9994980009210144e-01  5.02e-05
9.9998745011752632e-01  1.25e-05
The number of iterations : 8
```

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motivation

We observe a very slow convergence for $\int_0^{\pi/2} \cos(x)dx$ with the composite trapezoidal rule.

2	7.8539816339744828e-01	2.15e-01
4	9.4805944896851990e-01	5.19e-02
8	9.8711580097277540e-01	1.29e-02
16	9.9678517188616966e-01	3.21e-03
32	9.9919668048507226e-01	8.03e-04
64	9.9979919432001874e-01	2.01e-04
128	9.9994980009210144e-01	5.02e-05
256	9.9998745011752632e-01	1.25e-05
512	9.9999686253528774e-01	3.14e-06
1024	9.9999921563419114e-01	7.84e-07
2048	9.9999980390857179e-01	1.96e-07
4096	9.9999995097714434e-01	4.90e-08
8192	9.9999998774428667e-01	1.23e-08
16384	9.9999999693607278e-01	3.06e-09
32768	9.9999999923401672e-01	7.66e-10
65536	9.9999999980850662e-01	1.91e-10
131072	9.9999999995212607e-01	4.79e-11
262144	9.9999999998802369e-01	1.20e-11
524288	9.9999999999699174e-01	3.01e-12
1048576	9.9999999999924849e-01	7.52e-13

justification the extrapolation

The error expansion of the composite trapezoidal rule has only even powers of h. We apply the following theorem.

Theorem (the Euler-Maclaurin summation formula)

For $g \in C^{2m+2}[0, N]$ (g is sufficiently many times continuously differentiable over $[0, N]$):

$$\frac{1}{2}g(0) + g(1) + \cdots + g(N-1) + \frac{1}{2}g(N) = \int_0^N g(t)dt + \sum_{\ell=1}^{m} \frac{B_{2\ell}}{(2\ell)!}\left(g^{(2\ell-1)}(N) - g^{(2\ell-1)}(0)\right) + \frac{B_{2m+2}}{(2m+2)!}Ng^{(2m+2)}(\alpha),$$

where $\alpha \in [0, N]$ and where B_k are the Bernoulli numbers.

the connection with the trapezoidal rule

To see the connection with the composite trapezoidal rule, we make a change of coordinates:

$$[0, N] \rightarrow [a, b] : t \mapsto x = a + ht, \quad h = \frac{b-a}{N}, \quad dx = hdt,$$

so

$$\int_0^N g(t)dt = \int_a^b f(x)\frac{1}{h}dx.$$

To replace the derivatives of $g(t)$ in the equation of the theorem, we observe $g(t) = f(a + ht) = f(x)$ and apply the chain rule:

$$g'(t) = f'(x)h \quad \text{and for any } \ell : g^{(\ell)}(t) = f^{(\ell)}(x)h^{\ell}.$$

rewriting the formula

After executing the coordinate change,
the formula of the theorem turns into

$$
\begin{aligned}
&\frac{1}{2}f(a) + f(a+h) + \cdots + f(b-h) + \frac{1}{2}f(b) \\
&\qquad = \int_a^b f(x)\frac{1}{h}dx \\
&\qquad + \sum_{\ell=1}^{m} \frac{B_{2\ell}}{(2\ell)!} h^{2\ell-1} \left(f^{(2\ell-1)}(b) - f^{(2\ell-1)}(a) \right) \\
&\qquad + \frac{B_{2m+2}}{(2m+2)!} N h^{2m+2} f^{(2m+2)}(\beta), \quad \beta \in [a,b].
\end{aligned}
$$

the error formula

Multiplying by h, we obtain the error formula for the composite trapezoidal rule $T(h)$:

$$
\begin{aligned}
T(h) &= \int_a^b f(x)dx \\
&+ \sum_{\ell=1}^{m} \frac{B_{2\ell}}{(2\ell)!} h^{2\ell} \left(f^{(2\ell-1)}(b) - f^{(2\ell-1)}(a) \right) \\
&+ \frac{B_{2m+2}}{(2m+2)!} (Nh) h^{2m+2} f^{(2m+2)}(\beta).
\end{aligned}
$$

Observe that only even powers of h occur.

This justifies the extrapolation formula used in Romberg integration.

deriving the extrapolation formula

$$\begin{aligned} T(h) &= \int_a^b f(x)dx + C_1 h^2 + \cdots \\ T(h/2) &= \int_a^b f(x)dx + C_1 \frac{h^2}{4} + \cdots \end{aligned}$$

We eliminate C_1 by

$$\frac{4T(h/2) - T(h)}{4-1} = \int_a^b f(x)dx + O(h^4).$$

a triangular table

Define the table $R[i, j]$, for $i = 1, 2, \ldots, n$, and $j = 1, 2, \ldots, i$.

The first column $R[i, 1]$ is the result of the composite trapezoidal rule with i intervals.

For $j > 1$, we apply the formula:

$$R[i, j] = \frac{4^{j-1} R[i, j-1] - R[i-1, j-1]}{4^{j-1} - 1}, \quad i = j, j+1, \ldots, n.$$

The algorithm is called *Romberg integration*.

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a Julia function

```
"""
    function romberg(t::Array{Float64,1})

Applies extrapolation to the approximations in t,
t is a sequence of results of the composite
Trapezoidal rule.

Example:

    t = adaptrap(cos,0,pi/2,6)
    et = romberg(t);
"""
```

the function definition

```
function romberg(t::Array{Float64,1})
    n = length(t)
    et = zeros(n,n)
    et[:,1] = t
    for i = 2:n
        for j = 2:i
            r = 4^(j-1)
            r1 = r-1
            et[i,j] = (r*et[i,j-1] - et[i-1,j-1])/r1
        end
    end
    return et
end
```

running the program

```
The composite trapezoidal rule :
       2  7.8539816339744828e-01  2.15e-01
       4  9.4805944896851990e-01  5.19e-02
       8  9.8711580097277540e-01  1.29e-02
      16  9.9678517188616966e-01  3.21e-03
      32  9.9919668048507226e-01  8.03e-04
      64  9.9979919432001874e-01  2.01e-04

Romberg integration :
7.8539816339744828e-01  2.15e-01
1.0022798774922104e+00  2.28e-03
9.9999156547299273e-01  8.43e-06
1.0000000081440208e+00  8.14e-09
9.9999999999801692e-01  1.98e-12
1.0000000000000002e+00  2.22e-16
```

the progress of the extrapolation errors

```
Romberg integration :
7.853981633974828e-01  2.15e-01
1.002279877492210e+00  2.28e-03
9.999915654729927e-01  8.43e-06
1.000000008144020e+00  8.14e-09
9.999999999980169e-01  1.98e-12
1.000000000000000e+00  2.22e-16

Errors in the table
  2.15e-01
  5.19e-02  2.28e-03
  1.29e-02  1.35e-04  8.43e-06
  3.21e-03  8.30e-06  1.24e-07  8.14e-09
  8.03e-04  5.17e-07  1.90e-09  2.98e-11  1.98e-12
  2.01e-04  3.23e-08  2.96e-11  1.15e-13  1.78e-15  2.22e-16
```

an application of Romberg integration

Exercise 3: Consider $\displaystyle\int_0^1 \sin(\pi x) dx = \frac{2}{\pi}$.

1. Apply the composite trapezoidal rule for this problem, for $n = 1, 2, 4, 8, 16, 32, 64$, and 128 intervals. How accurate is the approximation for each n?
2. Apply Romberg integration to the computed approximations. How accurate is the final result?

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the composite trapezoidal rule on $\int_0^1 \sqrt{1-x^2}dx$

1	5.000000000000000e-01	2.85e-01
2	6.830127018922193e-01	1.02e-01
4	7.489272670256101e-01	3.65e-02
8	7.724547860892933e-01	1.29e-02
16	7.808132594569353e-01	4.58e-03
32	7.837756057192827e-01	1.62e-03
64	7.848242281949214e-01	5.74e-04
128	7.851951980991536e-01	2.03e-04
256	7.853263957393075e-01	7.18e-05
512	7.853727881799136e-01	2.54e-05
1024	7.853891916347549e-01	8.97e-06
2048	7.853949913528606e-01	3.17e-06
4096	7.853970419019397e-01	1.12e-06
8192	7.853977668874225e-01	3.97e-07
16384	7.853980232097232e-01	1.40e-07
32768	7.853981138335608e-01	4.96e-08
65536	7.853981458739598e-01	1.75e-08
131072	7.853981572019569e-01	6.20e-09
262144	7.853981612070172e-01	2.19e-09
524288	7.853981626230216e-01	7.74e-10
1048576	7.853981631236601e-01	2.74e-10

verifying the conditions for Romberg integration

Can we apply Romberg integration directly to $\displaystyle\int_0^1 \sqrt{1 - x^2} dx$?

The opening statement of the Euler-Maclaurin summation formula:

For $g \in C^{2m+2}[0, N]$ (g is sufficiently many times continuously differentiable over $[0, N]$):

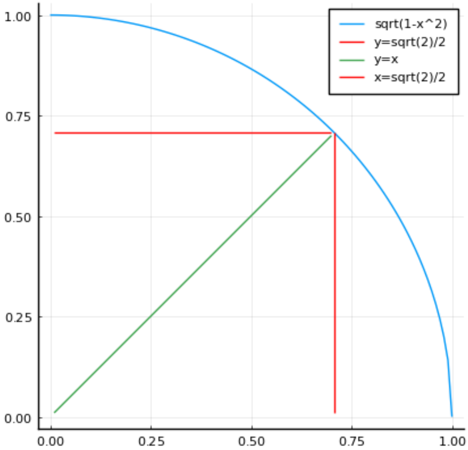
The first derivative of $\sqrt{1 - x^2}$ is $\dfrac{-x}{\sqrt{1 - x^2}}$

and $\dfrac{-x}{\sqrt{1 - x^2}}$ is not defined at $x = 1$.

Therefore, $\sqrt{1 - x^2}$ is not sufficiently many times continuously differentiable over $[0, 1]$.

Romberg integration will not give more accurate results!

reformulating the problem



Apply Romberg integration to $\displaystyle\int_0^{\sqrt{2}/2} \sqrt{1-x^2} - \frac{\sqrt{2}}{2} dx$.

Romberg integration on $\int_0^{\sqrt{2}/2} \sqrt{1-x^2} - \frac{\sqrt{2}}{2} dx$.

```
$ julia romberg4pi.jl
The composite trapezium rule :
       2  1.035533905932737e-01  3.91e-02
       4  1.324956091797106e-01  1.02e-02
       8  1.401101760318160e-01  2.59e-03
      16  1.420490393176905e-01  6.50e-04
      32  1.425363845687003e-01  1.63e-04
      64  1.426583955635967e-01  4.07e-05
Romberg integration :
1.035533905932737e-01  3.91e-02
1.421430153751896e-01  5.56e-04
1.426820549563396e-01  1.70e-05
1.426987182500889e-01  3.63e-07
1.426990777811069e-01  3.92e-09
1.426990816805300e-01  1.82e-11
```

comparing to $\int_0^{\sqrt{2}/2} \sqrt{1 - x^2} - \frac{\sqrt{2}}{2} dx = (\pi - 2)/8$

```
Romberg integration :
1.0355339059327372e-01  3.91e-02
1.4214301537518967e-01  5.56e-04
1.4268205495633965e-01  1.70e-05
1.4269871825008892e-01  3.63e-07
1.4269907778110696e-01  3.92e-09
1.4269908168053008e-01  1.82e-11
Errors in the table
  3.91e-02
  1.02e-02  5.56e-04
  2.59e-03  5.07e-05  1.70e-05
  6.50e-04  3.75e-06  6.24e-07  3.63e-07
  1.63e-04  2.49e-07  1.50e-08  5.32e-09  3.92e-09
  4.07e-05  1.58e-08  2.76e-10  4.27e-11  2.20e-11  1.82e-11
```

We get 10 decimal places accuracy with 64 instead of 1,048,576 intervals.

Romberg integration for π again

Exercise 4: Consider

$$\int_0^1 \frac{16x - 16}{x^4 - 2x^3 + 4x - 4} dx = \pi.$$

1. Apply the composite trapezoidal rule to this problem.
   How many function evaluations are needed to obtain 10 decimal places of accuracy?
2. Is the integrand sufficiently many times continuously differentiable over [0,1]? *Hint: compute the roots of the denominator.*
3. Applies Romberg integration to this problem.
   How many function evaluations are needed to obtain 10 decimal places of accuracy?

concluding remarks

- In an efficient organization of adaptive integration,
  the information of all previous function evaluations is used.
- Romberg integration applies extrapolation to improve the slow convergence of the composite Trapezoidal rule.

  The integrand must be sufficiently many times continuously differentiable over the interval,
  otherwise Romberg integration will not improve the accuracy.