16. Romberg Integration and Gaussian Quadratures

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Contents

1	Introduction
2	Richardson Extrapolation
	2.1 The Logic of the Richardson Method
	2.2 Algorithm of Richardson Method
	2.3 Higher Order Extrapolation
	2.4 Algorithm and Code
3	Romberg Integration
	3.1 Approximation formula and Error Analysis
	3.2 Romberg Algorithm
	3.3 R Code
4	Gaussian Quadrature
	4.1 Two-point Gauss Legendre Formula
	4.2 General Gauss Legendre Formula
	4.3 R Code
5	Remarks

1 Introduction

Interpolation is to estimate a value between a given set of known values. Extrapolation is to use of known values to project a value outside of the intended range of the previous values.

In trapezoid and Simpson's methods, the accuracy of the approximation increases as the step size h = (b-a)/n decreases (i.e., n gets bigger). From the computational perspective, reducing h requires increasing the number of points n, and so increases the "cost" (time and other resources needed) of the calculation.

https://github.com/pengdsci/MAT325/raw/main/w13/img/w13-trapezoid-sum.gif

In this note, we will introduce methods that use the same step size h but archives a more accurate approximation.

2 Richardson Extrapolation

Using the concept of Richardson Extrapolation, very higher-order integration can be achieved using only a series of values from the Trapezoidal Rule. Similarly, accurate values of derivatives could be obtained using low-order central difference derivatives.

2.1 The Logic of the Richardson Method

Assume that $\phi(h)$ is infinitely continuously differentiable as a function of h, thus allowing us to expand $\phi(h)$ in the Taylor series

$$\phi(h) = \phi(0) + h\phi'(0) + \frac{\phi''(0)}{2!}h^2 + \frac{\phi'''(0)}{3!}h^3 + \frac{\phi^{(4)}(0)}{4!}h^4 + O(h^5)$$

Let $c_i = \frac{\phi^{(i)}(0)}{i!}$. We rewrite the above Taylor expansion to get

$$\phi(h) = \phi(0) + c_1 h + c_2 h^2 + c_3 h^3 + c_4 h^4 + O(h^5)$$

Apparently,

$$\phi(h/2) = \phi(0) + \frac{c_1}{2}h + \frac{c_2}{4}h^2 + \frac{c_3}{8}h^3 + \frac{c_4}{16}h^4 + O(h^5)$$

Define $\psi(h) = 2\phi(h/2) - \phi(h)$. We have

$$\psi(h) = \phi(0) - \frac{c_2}{2}h^2 - \frac{3c_3}{4}h^3 - \frac{7c_4}{8}h^4 - O(h^5)$$

Note that $\psi(h)$ also approximates $\phi(0)$, but with an $O(h^2)$ error, rather than the O(h) error. For small h, this $O(h^2)$ approximation will be considerably more accurate.

If we repeat what we did on $\phi(x)$ to $\psi(x)$, that is

$$\psi(h/2) = \phi(0) - \frac{c_2}{8}h^2 - \frac{3c_3}{32}h^3 - \frac{7c_4}{128}h^4 - O(h^5)$$

To cancel the two terms that contain h^2 , we define $\psi_1(h) = [4\psi(h/2) - \psi(h)]/3$ in the following

$$\psi_1(h) = \phi(0) + \frac{4\psi(h/2) - \psi(h)}{3} = \frac{c_3}{8}h^3 + \frac{7c_4}{32}h^4 + O(h^5)$$

Similarly, $\psi_1(0) = \psi(0) = \phi(0)$ but the approximation $\psi_1(0)$ has an $O(h^3)$ error. This means $\psi_1(0)$ more accurate than $\psi(0)$.

We can continue this procedure repeatedly, each time improving the accuracy by one order, at the cost of one additional computation with a smaller h.

2.2 Algorithm of Richardson Method

To facilitate generalization and to avoid a further tangle of notations for developing an algorithm, we use two indices and define

$$R(j,0) := \phi(h/2^j)$$
 $j \ge 0;$ $R(j,k) := \frac{2^k R(j,k-1) - R(j-1,k-1)}{2^k - 1}$ $j \ge k > 0.$

This procedure is called Richardson extrapolation after the British applied mathematician Lewis Fry Richardson, a pioneer of the numerical solution of partial differential equations, weather modeling, and mathematical models in political science.

With the above notations, we summarize the previous derivation of various approximations of $\phi(0)$ in the following table.

R(0; 0) =
$$\phi(h)$$
,
R(1; 0) = $\phi(h/2)$, R(1; 1) = $\psi(h)$;
R(2; 0) = $\phi(h/2^2)$, R(2; 1) = $\psi(h/2)$, R(2; 2) = $\psi_1(h)$

In general, the recursive algorithm can be represented in the following triangular extrapolation table.

$$R(0,0)$$
 $R(1,0)$ $R(1,1)$
 $R(2,0)$ $R(2,1)$ $R(2,2)$
 $R(3,0)$ $R(3,1)$ $R(3,2)$ $R(3,3)$
 \dots \dots \dots order of $O(h)$ $O(h^2)$ $O(h^3)$ $O(h^4)$ error

Remarks:

- 1. We expect the bottom-right element in the table to be the most accurate approximation to $\phi(0)$.
- 2. The recursive process is built on the approximations in the first column (see the following flow chart).

$$\begin{array}{c} R(0,0) \\ R(1,0) \\ R(2,0) \\ R(3,0) \\ R(3,0) \\ R(3,1) \\ R(3,0) \\ R(3,1) \\ R(3,1) \\ R(3,1) \\ R(3,2) \\ R(3,2) \\ R(3,3) \\ R(3,3) \\ R(3,1) \\ R(3,2) \\ R(3,3) \\ R(3,3) \\ R(3,1) \\ R(3,2) \\ R(3,3) \\ R(3,3) \\ R(3,1) \\ R(3,1) \\ R(3,2) \\ R(3,3) \\ R(3,1) \\ R(3,1) \\ R(3,2) \\ R(3,3) \\ R(3,1) \\ R(3,1) \\ R(3,2) \\ R(3,1) \\ R(3,2) \\ R(3,2) \\ R(3,2) \\ R(3,2) \\ R(3,3) \\ R(3,2) \\ R(3,2) \\ R(3,3) \\ R(3,2) \\ R(3,3) \\ R(3,2) \\ R(3,3) \\ R(3,3) \\ R(3,2) \\ R(3,3) \\ R(3,2) \\ R(3,3) \\ R(3,2) \\ R(3,2) \\ R(3,3) \\ R(3,2) \\ R(3,3) \\ R(3,2) \\ R(3,2) \\ R(3,3) \\ R(3,2) \\ R(3,2$$

3. Each of the cells in the triangular table is a valid approximation of $\phi(0)$.

2.3 Higher Order Extrapolation

If the initial algorithm $\phi(h)$ is better than O(h) accurate and in this case the formula for R(j;k) should be adjusted to take advantage. That is, if

$$\phi(h) = \phi(0) + c_1 h^r + c_2 h^{2r} + c_3 h^{3r} + c_4 h^{4r} + O(h^{5r})$$

for some integer $x \geq 1$. For example,

$$\cos(h) = 1 - \frac{1}{2!}h^2 + \frac{1}{4!}h^{2\times 2} - \frac{1}{3!}h^{2\times 3}h^6 + O(h^{2\times 4})$$

where r=2.

We then can define the following recursive relationship below.

$$\begin{array}{lll} R(j,0) & := & \phi(h/2^j) & j \geq 0; \\ R(j,k) & := & \frac{2^{rk}R(j,k-1)-R(j-1,k-1)}{2^{rk}-1} & j \geq k > 0. \end{array}$$

The corresponding extrapolation table is given by

2.4 Algorithm and Code

The recursive extrapolation procedure itself is simple arithmetic. It is easy to make a R/MATLAB function to implement the algorithm.

Example 1: Let $f(x) = \exp(x)$. Find f'(1) with h = 1.

Solution Define

$$\phi(h) = \frac{f(1+h) - f(1)}{h}$$

Then $f'(1) = \lim_{h\to 0} \phi(h) = f'(1)$. We use Richardson extrapolation to approximate f'(1).

```
fn = function(h) (exp(1+h)-exp(1))/h
Richardson.Method(fn, h=1, r=1, digit=8, J=7)
                                  [,3]
                       [,2]
                                            [,4]
##
                                                      [,5]
                                                                 [,6]
                                                                           [,7]
## [1,] 4.6707743
## [2,] 3.5268145 2.3828547
## [3,] 3.0882445 2.6496745 2.7386145
## [4,] 2.8954802 2.7027158 2.7203962 2.7177936
## [5,] 2.8050259 2.7145715 2.7185234 2.7182559 2.7182867
## [6,] 2.7612009 2.7173759 2.7183107 2.7182803 2.7182820 2.7182818
## [7,] 2.7396294 2.7180580 2.7182854 2.7182817 2.7182818 2.7182818 2.7182818
```

Example 2. Find the first order derivative of $f(x) = x * \exp(x)$ at x = 2 with h = 1/2. The true value is $f'(2) = 2 + 2 \exp(2)$.

Solution: To use the Richardson method, we define

$$\phi(h) = \frac{f(2+h) - f(2)}{h}$$

```
fn = function(h) ((2+h)*exp(2+h)-(2)*exp(2))/(h)
Richardson.Method(fn, h=1/2, r=1, digit=8, J=5)

##     [,1]     [,2]     [,3]     [,4]     [,5]

## [1,] 31.356245

## [2,] 26.277174 21.198102

## [3,] 24.114360 21.951546 22.202694

## [4,] 23.115311 22.116262 22.171167 22.166664

## [5,] 22.635054 22.154798 22.167643 22.167171
```

3 Romberg Integration

The Romberg integration uses the Richardson extrapolation on the composite trapezoidal rule.

3.1 Approximation formula and Error Analysis

Recall that, if f(x) is in $C^{\infty}[a,b]$ (i.e., any given order of derivative of f(x) exists and is continuous), the composite trapezoid rule approximates the integral $\int_a^b f(x)dx$ by

$$\int_{a}^{b} f(x)dx \approx \frac{h}{2} \left[f(a) + 2 \sum_{j=1}^{n-1} f(a+jh) + f(b) \right]$$

where h = (b - a)/n. n is the number of sub-intervals. The error term given in the previous note can be written as

$$E = \sum_{i=1}^{n} E_i = \sum_{i=1}^{n} \int_{x_i}^{x_{i+1}} \left[f(x) - S(x) \right] dx = \sum_{i=1}^{n} \frac{f''(c_i)}{2} \times \left[-\frac{(x_{i+1} - x_i)^3}{6} \right]$$
 (see the last note)

$$= \sum_{i=1}^{n} \frac{f''(c_i)}{n} \times \left[-\frac{n(x_{i+1} - x_i)^3}{12} \right] = -\frac{nh^3}{12} \sum_{i=1}^{n} \frac{f''(c_i)}{n}.$$

where c_i is a number in subinterval $[x_i, x_{i+1}]$. Clearly for i = 1, ..., n,

$$\min_{x \in [a,b]} f''(x) \le f''(c_i) \le \max_{x \in [a,b]} f''(x).$$

Therefore,

$$\min_{x \in [a,b]} f''(x) \le \frac{\sum_{i=1}^{n} f''(c_i)}{n} \le \max_{x \in [a,b]} f''(x).$$

By the intermediate mean value theorem, there exists a value in [a, b], say ξ , such that

$$f''(\xi) = \sum_{i=1}^{n} \frac{f''(c_i)}{n}$$

Therefore,

$$E = \sum_{i=1}^{n} E_i = -\frac{nh^3}{12} \sum_{i=1}^{n} \frac{f''(c_i)}{n} = -\frac{nh^3}{12} f''(\xi) = -\frac{(b-a)f''(\xi)}{12} h^2.$$

The complete expression of the numerical integration using the trapezoid rule with n-subintervals is given by

$$T(h) = \int_{a}^{b} f(x)dx = \frac{h}{2} \left[f(a) + 2\sum_{j=1}^{n-1} f(a+jh) + f(b) \right] - \frac{(b-a)f''(\xi)}{12}h^{2}$$

where $a = x_0 < x_1 < \cdots < x_n = b$. $\{x_1, \cdots, x_n\}$ are equal spaced and h = (b - a)/n. c_i is in [a, b].

3.2 Romberg Algorithm

From the last formula of the previous sub-section, we see that the trapezoidal rule has an order of approximation $O(h^2)$. Therefore, following the Richardson extrapolation with r=2, we have

$$R(j,0) = T(h/2^j)$$
 for $j \ge 0$
$$R(j,k) = \frac{4^k R(j,k-1) - R(j-1,k-1)}{4^k - 1}$$
 for $j \ge k > 0$.

The corresponding Richardson extrapolation table is given by

3.3 R Code

Since this is a direct application of the Richardson extrapolation. We will simply implement it in R.

```
Romberg.Trapz = function(fn,
                                  # The original function f(x)
                                  # lower limit of the given interval
                                  # upper limit of the given interval
                         r = 2, # 2nd order approximation error for the trapezoid
                         dec = 7, # number of digits in the output
                                  # order of Richardson extrapolation
                         J
                         ){
   ## Trapezoid rule
  h = b - a
                   # initial h
   Trapz.fn = function(a,b,h){
                   X = seq(a,b,h)
                   TP = h*sum(fn(X)) - h*(fn(a)+fn(b))/2
                   TP
                  }
   ## Romberg Int. starts:
  RR = matrix(rep(NA,J^2), ncol=J)
  for (i in 1:J) RR[i,1] = Trapz.fn(a,b, h/2^(i-1)) ## defining R(j,0)
   for (k in 2:J){
       for (j in k:J){
           RR[j,k]=(2^{(r*(k-1))*}RR[j,k-1]-RR[j-1, k-1])/(2^{(r*(k-1))-1})
     }
   options(digits = dec)
  print(RR, na.print = "")
}
```

Example 4: Find the approximation of the integral

$$\int_0^{\pi} \sin(x) dx$$

Solution: We first use the Romberg method.

```
fn = function(x) sin(x)
Romberg.Trapz(fn, a = 0, b = pi, r = 2, dec = 8, J = 5)
##
                  [,1]
                            [,2]
                                       [,3]
                                                 [,4] [,5]
## [1,] 1.9236072e-16
## [2,] 1.5707963e+00 2.0943951
## [3,] 1.8961189e+00 2.0045598 1.9985707
## [4,] 1.9742316e+00 2.0002692 1.9999831 2.0000055
## [5,] 1.9935703e+00 2.0000166 1.9999998 2.0000000
We can also print out the error of approximation in the following (not that the value of the integral is 2)
print(2-Romberg.Trapz(fn, a = 0, b = pi, r = 2, dec = 8, J = 6), na.print = "")
##
                            [,2]
                                      [,3]
                                                 [,4] [,5] [,6]
                  [,1]
## [1,] 1.9236072e-16
## [2,] 1.5707963e+00 2.0943951
## [3,] 1.8961189e+00 2.0045598 1.9985707
## [4,] 1.9742316e+00 2.0002692 1.9999831 2.0000055
## [5,] 1.9935703e+00 2.0000166 1.9999998 2.0000000
## [6,] 1.9983934e+00 2.0000010 2.0000000 2.0000000
                                                              2
```

```
[,2]
                                              [,3]
                                                              [,4]
                                                                            [,5]
##
                [,1]
## [1,] 2.0000000000
## [2,] 0.4292036732 -9.4395102e-02
## [3,] 0.1038811021 -4.5597550e-03 1.4292682e-03
## [4,] 0.0257683981 -2.6916995e-04 1.6869054e-05 -5.5499797e-06
## [5,] 0.0064296562 -1.6591048e-05 2.4754543e-07 -1.6288042e-08 5.4127094e-09
## [6,] 0.0016066390 -1.0333694e-06 3.8091554e-09 -5.9674488e-11 3.9661607e-12
##
                  [,6]
## [1,]
## [2,]
## [3,]
## [4,]
## [5,]
## [6,] -1.3207213e-12
```

In the above example, the error for **Romberg approximation** using the composite trapezoidal rule with 16 $(= 2^4)$ intervals is about 10^{-9} (level 5).

Next, we use the trapezoid method to approximate the integral and calculate absolute error in the following (the R function is copied from the previous note).

```
Trapezoid.int = function(fun,
                                         # fun = user-defined function
                                        # interval [a, b]
                          xvec,
                                        # number of partitions
                          n = 1,
                          graph=TRUE){ # request graphical representation
  a = min(xvec)
  b = max(xvec)
  m = length(xvec)
  if (n \ge m) xvec = seq(a,b,(b-a)/n)
  yvec = fun(xvec)
  nn = length(yvec)
  h = xvec[-1] - xvec[-nn]
  y.adjacent.sum = yvec[-1] + yvec[-nn]
  Iab = sum(h*y.adjacent.sum)/2
  if(graph == TRUE){
      x.margin = 0.1*abs(b-a)
      tt = seq(a-x.margin, b+x.margin, (b-a+2*x.margin)/10<sup>4</sup>)
      \lim x = c(a-x.margin, b+x.margin)
      y.max = max(fun(tt))
      y.min = min(fun(tt))
      y.margin = 0.1*abs(y.max-y.min)
      \lim_{y \to c} y = c(y.\min - y.margin, y.max + y.margin)
      plot(tt, fun(tt), type="l", col="blue", xlim=lim.x, ylim=lim.y, xlab=" ",ylab="")
      title("Trapezoidal Rule")
      lines(xvec, yvec, type="l", col="red")
      points(xvec, yvec, pch=21, col="red", cex = 0.6)
    }
  Iab
}
fun = function(x) sin(x)
2 - Trapezoid.int(fun=fun, xvec=c(0,pi), n = 15000, graph=FALSE)
```

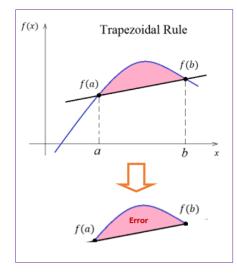
[1] 7.3108182e-09

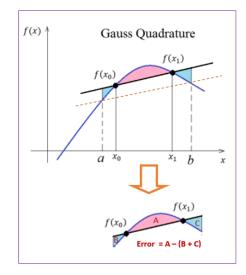
To obtain the same approximation error, the trapezoid method requires about 15000 intervals. That is, the

step size $h = \pi/15000 \approx 0.00021$. In the Romberg approach, the step size is $h = \pi/16 \approx 0.196$. The Romberg approach certainly saves a significant amount of computational time.

4 Gaussian Quadrature

The accuracy of numerical integration can be improved by choosing the sampling points wisely (not necessarily to be equally spaced). For example, consider the approximation of $\int_a^b f(x)dx$ in the following figure, the left panel represents the trapezoid approximation with an approximation error being represented as the area of the pink region. We can search two points x_0 and x_1 in the neighborhood a and b respectively such that $A \approx C + B$ (see the right panel in the following figure), we will then get a slightly bigger trapezoid (defined on the same interval [a, b] as that in the regular trapezoid approximation). The resulting approximation error is approximately equal to A - (C + B) which is significantly more accurate than the trapezoid approximation.





Recall that the area under the straight line, generated by the trapezoidal rule, can be expressed as

$$I_T = \frac{b-a}{2}[f(a) + f(b)] = \frac{b-a}{2}f(a) + \frac{b-a}{2}f(b) = \alpha_0 f(a) + \beta_0 f(b)$$

where $\alpha_0 = \beta_0 = (b-a)/2$. The objective of the Gauss quadrature is to fit the straight line, through two points $(x_0, f(x_0))$ and $(x_1, f(x_1))$, such that the area

$$I_G = \alpha f(x_0) + \beta f(x_1)$$

is exactly when the function f(x) being integrated is linear or constant. Next, we derive the Gauss quadrature approximation formula.

4.1 Two-point Gauss Legendre Formula

Since there are four parameters $(\alpha, \beta, x_0, x_1)$ in I_G to determine, we need to have four equations based on the assumption that I_G is approximated by its true integral based on the four basis polynomials $\{1 = x^0, x_1, x^2, x^3\}$. To be more specific,

1.
$$f(x) = K$$
 (constant function), $I_G = \alpha K + \beta K = \int_a^b K dx = K(b-a) \Rightarrow \alpha + \beta = b-a$.

2.
$$f(x) = Kx$$
: $I_G = \alpha Kx_0 + \beta Kx_1 = \int_a^b Kx dx = K(b^2 - a^2)/2 \Rightarrow \alpha x_0 + \beta x_1 = (b^2 - a^2)/2$.

3.
$$f(x) = Kx^2$$
: $I_G = \alpha Kx_0^2 + \beta Kx_1^2 = \int_a^b Kx^2 dx = K(b^3 - a^3)/3 \Rightarrow \alpha x_0^2 + \beta x_1^2 = (b^3 - a^3)/3$.

4.
$$f(x) = Kx^3$$
: $I_G = \alpha Kx_0^3 + \beta Kx_1^3 = \int_a^b Kx^3 dx = K(b^4 - a^4)/4 \Rightarrow \alpha x_0^3 + \beta x_1^3 = (b^4 - a^4)/4$.

After some algebra, we can find the solution to the following non-linear equation

$$\alpha + \beta = a - b
\alpha x_0 + \beta x_1 = (a^2 - b^2)/2
\alpha x_0^2 + \beta x_1^2 = (a^3 - b^3)/3
\alpha x_0^3 + \beta x_1^3 = (a^4 - b^4)/4$$

that satisfies $x_0 < x_1$ and a < b has the following form

$$\begin{array}{rcl} x_0 & = & (a+b)/2 - \sqrt{3}(b-a)/6 \\ x_1 & = & (a+b)/2 + \sqrt{3}(b-a)/6 \\ \alpha & = & (b-a)/2 \\ \beta & = & (b-a)/2 \end{array}$$

Therefore, the two-points Gauss-Legendre formula is given by

$$I_G = \frac{b-a}{2} \left\{ f \left[\frac{a+b}{2} - \frac{\sqrt{3}}{6} (b-a) \right] + f \left[\frac{a+b}{2} + \frac{\sqrt{3}}{6} (b-a) \right] \right\}$$

4.2 General Gauss Legendre Formula

Consider the general case of n segments with step size h = (b-a)/n. For $I_G^{(k)}$ on $[x_k, x_{k+1}]$, $h = x_{k+1} - x_k$ and $x_k + x_{k+1} = [a + (k-1)h] + [a + kh] = 2a + (2k-1)h$. that is,

$$I_G^{(k)} = \frac{x_{k+1} - x_k}{2} \left\{ f \left[\frac{x_k + x_{k+1}}{2} - \frac{\sqrt{3}}{6} (x_{k+1} - x_k) \right] + f \left[\frac{x_k + x_{k+1}}{2} + \frac{\sqrt{3}}{6} (x_{k+1} - x_k) \right] \right\}$$

$$= \frac{h}{2} \left\{ f \left[\frac{2a + (2k - 1)h}{2} - \frac{\sqrt{3}}{6}h \right] + f \left[\frac{2a + (2k - 1)h}{2} + \frac{\sqrt{3}}{6}h \right] \right\}$$

$$= \frac{h}{2} \left\{ f \left[a + \left(k - \frac{3 + \sqrt{3}}{6} \right) h \right] + f \left[a + \left(k - \frac{3 - \sqrt{3}}{6} \right) h \right] \right\}$$

Therefore,

$$I_G = \sum_{k=1}^n I_G^{(k)} = \frac{h}{2} \sum_{k=1}^n \left\{ f \left[a + \left(k - \frac{3 + \sqrt{3}}{6} \right) h \right] + f \left[a + \left(k - \frac{3 - \sqrt{3}}{6} \right) h \right] \right\}.$$

4.3 R Code

We convert the above formula to an R function in the following.

```
fn = function(x) sin(sin(x))
Gauss.Quadrature(fn=fn, a = 1, b = 2, n = 10)
```

[1] 0.81644998

Example: Consider integral

$$\int_{1}^{3} [x^{6} - x^{2} \sin(2x)] dx \approx 317.20236$$

The Gauss Quadrature approximation with n = 3 gives the following approximated value

```
fn = function(x) x^6 - x^2*sin(2*x)

Gauss.Quadrature(fn=fn, a = 1, b = 3, n = 3)
```

[1] 317.20203

5 Remarks

We make several remarks to conclude this note.

- 1. The analysis of the error of Gauss Legendre is out of the scope of this course. We will not discuss error bound or the order of approximation.
- 2. There are built-in functions in both R and MATLAB that implement Gauss quadrature.