

Exercises Lecture V Numerical Integration in 1D

1. Equispaced points: comparison trapezoidal-Simpson rules

Consider the definite integral :

$$I = \int_0^1 e^x dx = e - 1 = 1.718282 \dots$$

- (a) Write a code (e.g. `int.f90`) to calculate the integral using the (1) trapezoidal rule or (2) the Simpson rule. In general, we indicate with F_n the estimate of the integral from x_0 to x_n using a discretisation in n intervals (even for the Simpson algorithm) of width $h = \frac{x_n - x_0}{n}$. Therefore:

$$\int_{x_0}^{x_n} f(x) dx = F_n^{trap} + \mathcal{O}(h^2) = F_n^{Simpson} + \mathcal{O}(h^4)$$

where

$$F_n^{trap} = h \left[\frac{1}{2} f_0 + f_1 + \dots + f_{n-1} + \frac{1}{2} f_n \right]$$

and

$$F_n^{Simpson} = h \left[\frac{1}{3} f_0 + \frac{4}{3} f_1 + \frac{2}{3} f_2 + \frac{4}{3} f_3 + \dots + \frac{4}{3} f_{n-3} + \frac{2}{3} f_{n-2} + \frac{4}{3} f_{n-1} + \frac{1}{3} f_n \right]$$

- (b) Which is the dependence on n of the error $\Delta_n = F_n - I$? You can choose $n = 2^k$ (with $k = 2, \dots, 8$, at least) in order to have equispaced points when doing a log-log plot. You should find $\Delta_n \approx 1/n^2$ for the *trapezoidal rule* and $\Delta_n \approx 1/n^4$ for the *Simpson rule*.

2. **Monte Carlo method:**
generic sample mean and importance sampling

- (a) Write a code to compute the numerical estimate F_n of $I = \int_0^1 e^{-x^2} dx = \frac{\sqrt{\pi}}{2} \operatorname{erf}(1) \approx 0.746824$ with the MC *sample mean* method using a set $\{x_i\}$ of n random points uniformly distributed in $[0,1]$:

$$F_n = \frac{1}{n} \sum_{i=1}^n f(x_i)$$

- (b) Write a code (a different one, or, better, a unique code with an option) to compute F_n using the *importance sampling* with a set $\{x_i\}$ of points generated according to the distribution $p(x) = Ae^{-x}$ (*Notice that erf is an intrinsic fortran function; useful to compare the numerical result with the true value*). Remind that in the *importance sampling* approach:

$$\int_a^b f(x)dx = \left\langle \frac{f(x)}{p(x)} \right\rangle \int_a^b p(x)dx \approx \frac{1}{n} \sum_{i=1}^n \frac{f(x_i)}{p(x_i)} \int_a^b p(x)dx = F_n$$

with $p(x)$ which approximates the behaviour of $f(x)$, and the average is calculated over the random points $\{x_i\}$ with distribution $p(x)$.

Notes: pay attention to:

- the normalization of $p(x)$;
- the exponential distribution: `expdev` provides random numbers x distributed in $[0, +\infty[$; here we need x in $[0, 1]$...

- (c) Compare the efficiency of the two sampling methods (uniform and importance sampling) for the estimate of the integral by calculating the following quantities: F_n , $\sigma_n = (\langle f_i^2 \rangle - \langle f_i \rangle^2)^{1/2}$, σ_n/\sqrt{n} , where $f_i = f(x_i)$ in the first case, and $f_i = \frac{f(x_i)}{p(x_i)} \int_a^b p(x)dx$ in the second case (make a log-log plot of the error as a function of n : what do you see?).

3. **MC Method: acceptance-rejection**

Using the acceptance-rejection method, calculate $\pi = 4I$ with $I = \int_0^1 \sqrt{1-x^2} dx$.

The numerical estimate of the integral is $F_n = \frac{n_s}{n}$ where n_s is the number of points under the curve $f(x) = \sqrt{1-x^2}$, and n the total number of points generated. An example is given in `pi.f90`. Estimate the error associated, i.e. the difference between F_n and the true value. Discuss the dependence of the error on n .

(*Notice that many points are needed to see the $n^{-1/2}$ behavior, which can be hidden by stochastic fluctuations; it is easier to see it by averaging over many results (obtained from random numbers sequences with different seeds)*)

4. **MC method–sample mean (generic); error analysis using the “average of the averages” and the “block average”** NOTE: THIS EXERCISE IS VERY IMPORTANT !!!

- (a) Write a code to estimate the same integral of previous exercise, $\pi = 4I$ with $I = \int_0^1 \sqrt{1-x^2} dx$, using the MC method of sample mean with uniformly distributed random points. Evaluate the error $\Delta_n = F_n - I$ for $n=10^2, 10^3, 10^4$: it should have a $1/\sqrt{n}$ behaviour.
- (b) Choose in particular $n = 10^4$ and consider the corresponding error Δ_n . Calculate $\sigma_n^2 = \langle f^2 \rangle - \langle f \rangle^2$. You should recognize that σ_n CANNOT BE CONSIDERED A GOOD ESTIMATE OF THE ERROR (it's much larger than the actual error...)
- (c) In order to improve the error estimate, apply the following two different methods of variance reduction: 1) “average of the averages”: do $m = 10$ runs with n points each, and consider the average of the averages and its standard deviation:

$$\sigma_m^2 = \langle M^2 \rangle - \langle M \rangle^2$$

where

$$\langle M \rangle = \frac{1}{m} \sum_{\alpha=1}^m M_{\alpha} \quad e \quad \langle M^2 \rangle = \frac{1}{m} \sum_{\alpha=1}^m M_{\alpha}^2$$

and M_{α} is the average of each run. You should recognize that σ_m is a good estimate of the error associated to each measurement (=each run) and $\sigma_m \approx \sigma_n/\sqrt{n}$ is the error associated to the average over the different runs.

- (d) 2) Divide now the $n = 10,000$ points into 10 subsets. Consider the averages f_s within the individual subsets and the standard deviation if the average over the subsets:

$$\sigma_s^2 = \langle f_s^2 \rangle - \langle f_s \rangle^2 .$$

You should notice that $\sigma_s/\sqrt{s} \approx \sigma_m$.

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!CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
!   int.f90:
!   integrates f(x)=exp(x) in the interval [vmin,vamx]=[0,1]
!   using trapezoidal and Simpson rule
!CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

module intmod
  public :: f, trapez, simpson
contains

  ! function to be integrated
  !
  function f(x)
    implicit none
    real :: f
    real, intent(in) :: x
    f = exp(x)
    return
  end function f

  ! trapezoidal rule
  !
  function trapez(i, min, max)
    implicit none
    real :: trapez
    integer, intent(in) :: i
    real, intent(in) :: min, max
    integer :: n
    real :: x, interval
    trapez = 0.
    interval= ((max-min) / (i-1))
    ! sum over the internal points (extrema excluded)
    do n = 2, i-1
      x = interval * (n-1)
      trapez = trapez + f(x) * interval
    end do
    ! add extrema
    trapez = trapez + 0.5 * (f(min)+f(max)) * interval
    return
  end function trapez

  ! Simpson rule
  !
  function simpson(i, min, max)
    implicit none
    real :: simpson

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integer, intent(in) :: i
real, intent(in) :: min, max
integer :: n
real :: x, interval
simpson = 0.
interval = ((max-min) / (i-1))
! loop EVEN points
do n = 2, i-1, 2
    x = interval * (n-1)
    simpson = simpson + 4*f(x)
end do
! loop ODD points
do n = 3, i-1, 2
    x = interval * (n-1)
    simpson = simpson + 2*f(x)
end do
! add extrema
simpson = simpson + f(min)+f(max)
simpson = simpson * interval/3
return
end function simpson

end module intmod

program int
use intmod
!
! variable declaration
!   accuracy limit
!   min and max in x
!
implicit none
real :: r1, r2, theo, vmin, vmax
integer :: i, n
! exact value
vmin = 0.0
vmax = 1.0
theo = exp(vmax)-exp(vmin)
print*, ' exact value =',theo
open(unit=7,file='int-tra-sim.dat',status='unknown')
!
write(7,*)"# N, interval, exact, Trap-exact, Simpson-exact"
do i = 2,8
    n = 2**i
    r1 = trapez(n+1, vmin, vmax)
    r1 = (r1-theo)

```

