Exercise Lecture VI: again on classical numerical integration (gaussian quadrature); gaussian distribution and central limit theorem

1. **1D "classical" integration: Gaussian Quadrature**

   Remind the Gauss-Legendre rule for *quadrature* with non equispaced points:

   $$\int_a^b f(x)dx \approx \sum_{i=1}^{n} w(i)f(x(i))$$

   For integration in [-1,1], x_i are the roots of the Legendre polynomials: abscissas and weights up to the fourth order, and the degree of the polynomial exactly integrable are listed in the following tables:

n	i	x_i	w_i	degree
1	1	0	2	1
2	1	-0.577350269189626	1	3
	2	0.577350269189626	1	
3	1	-0.774596669241483	0.555555555555556	5
	2	0	0.888888888888889	
	3	0.774596669241483	0.555555555555556	
4	1	-0.861136311594053	0.347854845137454	7
	2	-0.339981043584856	0.652145154862546	
	3	0.339981043584856	0.652145154862546	
	4	0.861136311594053	0.347854845137454	

   We can transform the special points and weights for integration in an arbitrary interval $[a, b]$ with the substitution ("new" refers to $[a, b]$, "old" to $[-1, 1]$):

   $$x_{new} = \frac{b-a}{2}x_{old} + \frac{b+a}{2} \qquad \text{and} \qquad w_{new} = \frac{b-a}{2}w_{old}$$

(a) Consider once again the definite integral

$$I = \int_0^1 e^x \; dx = e - 1$$

whose numerical estimate F_N has been already calculated using (1) the trapezoidal and (2) the Simpson's rule in the previous exercise session. Now we use (3) the Gauss-Legendre quadrature. Here is listed a simple program implementing explicitly the second-order formula (`gauleg-IIorder.f90`). Verify that already at this order, the Gauss-Legendre quadrature gives a very good approximation.

(b) A more general implementation of Gauss-Legendre is proposed in `gauleg-other.f90` which makes use of the subroutine `gauleg` from "Numerical Recipes" (but the code is self-contained, it can be used without any external routine/module/interface). Estimate the relative error

$$\epsilon = \left| \frac{numeric - exact}{exact} \right|$$

for the 3 different methods, considering e.g. N=2, 4, 8, 16, 32, 64. Make a log-log plot of $|\epsilon|$ as a function of N. What about the dependence of the error on N? Can you identify the range of N where the roundoff errors are dominant? (consider the possibility of increasing the precision).

(c) The program `gauleg_nr_test.f90` is another example of the use of the subroutine `gauleg` from "Numerical Recipes"; where the subroutine and other auxiliary routines/module/interface are external and must be compiled and linked. They are extracted from the "Numerical Recipes" library, properly simplified (the original versions contain more and more subroutines) and are listed at the end of these notes.

In order to use the routines of Numerical Recipes, you have to compile and link the main program with:
- the subroutine `gauleg` which gives points and abscissas
- `nrtype.f90` containing type declarations; - `nrutil.f90` containing modules and utilities; - `nr.f90` containing (through a module with `interfaces`) the conventions to call the subroutines with the main program

You must compile these files with the option `-c`: this produces `.mod` and `.o` (the objects). In a second step compile the main program. Finally you link all the files `.o` and produce the executable:

```
g95 -c nrtype.f90 nrutil.f90 nr.f90 gauleg.f90
g95 -c gauleg_nr_test.f90
g95 -o a.out gauleg_nr_test.o nrtype.o nrutil.o nr.o gauleg.o
```

2. **Random numbers with gaussian distribution: the central limit theorem**
Use the central limit theorem in order to produce random numbers with gaussian distribution. Remind that given a sequence of independent random numbers r_i, their average

$$x_N = \frac{1}{N} \sum_{i=1}^{N} r_i$$

is distributed according to

$$P_N(x) = \frac{1}{\sqrt{2\pi\sigma^2}} exp\left(-\frac{(x_N - \mu)^2}{2\sigma^2}\right)$$

with $\mu =< r >$, $\sigma^2 = (< r^2 > - < r >^2)/N$.
Furthermore, defining

$$z_N = \frac{x_N - \mu}{\sigma}$$

we have $< z_N^4 >\approx 3 < z_N^2 >^2$.

   (a) Use random numbers r_i uniformly distributed in [−1,1], choosing N≈ 500 and generating at least ≈ 100 points x_N. Verify (doing an histogram) that x_N have a Gaussian distribution.

   (b) Calculate numerically $< x_N >$ and σ_x^2 and compare them with μ and σ^2 analytically calculated.

   (c) Consider z_N and verify numerically the relationship $< z_N^4 >\approx 3 < z_N^2 >^2$.

   (d) Do again the exercise using random numbers r_i with exponential distribution ($p(r) = e^{-r}$ if $r \geq 0$, 0 elsewhere). Calculate $< x_N >$, $\sigma_{x_N}^2$ and μ, σ^2 numerically and analytically, respectively.

   (e) Consider now random numbers r_i with distribution

$$p(r) = \frac{a}{\pi} \frac{1}{r^2 + a^2}$$

   (Lorentz's), with $a = 1$, for instance. Do $\langle x \rangle$, $\langle x^2 \rangle$ and σ_x^2 exist?? Try to determine the characteristic of the distribution of the variable sum $x_N = \frac{1}{N} \sum_{i=1}^{N} r_i$.

```
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
!  gauleg-IIorder.f90
!  test Gauss-Legendre quadrature II-order formula in the interval (a,b);
!  Here: integrand function is f(x)=exp(x), but it is easy to change
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

module gaussint
  public :: f
contains

  function f(X)
    ! integrand function
    implicit none
    real :: f
    real, intent(in) :: X
    F=exp(x)
  end function f

  subroutine gausquad(f,a,b,estimate)
    real :: f
    real, intent(in) :: a,b
    real, intent(out) :: estimate
        estimate=(b-a)/2*((f(-(b-a)/2/sqrt(3.)+(b+a)/2.)+f((b-a)/2/sqrt(3.)+(b+a)/2.)))
  end subroutine gausquad

end module gaussint

program gauleg_test
  use gaussint
  implicit none
  real :: a,b,estimate, exact
  character :: answ*1
  integer :: J
  write(*,*)' Gauss-Legendre II-order quadrature for exp(x) in [a,b] interval:'
  write(*,*)' Int( F(X) DX  )~  SUM_(k=1)^N w_k F(x_k ) '
10 write(*,*)' insert a, b > '
  read (*,*) a,b
  call GAUSQUAD(f,a,b,estimate)
  write(*,*)' exact value        : ',exp(b)-exp(a)
  write(*,*)' numerical estimate : ', estimate
  write(*,*)' error              : ', estimate-(exp(b)-exp(a))
  write(*,*)' other interval ? <Y/N> '
  read (*,'(A)') answ
  if (answ=='Y' .or. answ=='y') goto 10
  stop
end program gauleg_test
```

```
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
! gauleg-other.f90     P145 Numerical Recipes in Fortran
! adapted from www.cs.umbbc.edu/~squire/download/gauleg.f90
! (everything self-contained!)
! compute x(i) and w(i)  i=1,n  Legendre ordinates and weights in (-1,1)
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

subroutine gaulegf(x1, x2, x, w, n)
  implicit none
  integer, intent(in) :: n
  double precision, intent(in) :: x1, x2
  double precision, dimension(n), intent(out) :: x, w
  integer :: i, j, m
  double precision :: p1, p2, p3, pp, xl, xm, z, z1
  double precision, parameter :: eps=3.d-14

  m = (n+1)/2
  xm = 0.5d0*(x2+x1)
  xl = 0.5d0*(x2-x1)
  do i=1,m
    z = cos(3.141592654d0*(i-0.25d0)/(n+0.5d0))
    z1 = 0.0
    do while(abs(z-z1) > eps)
      p1 = 1.0d0
      p2 = 0.0d0
      do j=1,n
        p3 = p2
        p2 = p1
        p1 = ((2.0d0*j-1.0d0)*z*p2-(j-1.0d0)*p3)/j
      end do
      pp = n*(z*p1-p2)/(z*z-1.0d0)
      z1 = z
      z = z1 - p1/pp
    end do
    x(i) = xm - xl*z
    x(n+1-i) = xm + xl*z
    w(i) = (2.0d0*xl)/((1.0d0-z*z)*pp*pp)
    w(n+1-i) = w(i)
  end do
end subroutine gaulegf

program gauleg
  implicit none
  integer :: i, j
  double precision, dimension(100) :: x, w
  double precision :: sum, a, b
```

```
  integer, parameter :: debug=0

  print *, 'test gauleg.f90 on interval -1.0 to 1.0 ordinates, weights'
  do i=1,15
    call gaulegf(-1.0d0, 1.0d0, x, w, i)
    sum = 0.0d0
    do j=1,i
      print *, 'x(',j,')=', x(j), '  w(',j,')=', w(j)
      sum = sum + w(j)
    end do
    print *, '             integrate(1.0, from -1.0 to 1.0)= ', sum
  print *, ' '
  end do

  a = 0.5d0
  b = 1.0d0
  print *, 'test gauleg on integral(sin(x), from ',a,' to ',b,')'
  do i=2,10
    call gaulegf(a, b, x, w, i)
    sum = 0.0d0
    do j=1,i
      if(debug>0)print *, 'x(',j,')=', x(j), '  w(',j,')=', w(j)
      sum = sum +w(j)*sin(x(j))
    end do
    print *, i, ' integral (0.5,1.0) sin(x) dx = ', sum
  end do
  print *, '-cos(1.0)+cos(0.5) =', -cos(b)+cos(a)
  print *, 'exact should be: 0.3372802560'
  print *, ' '

  a = 0.5d0
  b = 5.0d0
  print *, 'test gauleg on integral(exp(x), from ',a,' to ',b,')'
  do i=2,10
    call gaulegf(a, b, x, w, i)
    sum = 0.0d0
    do j=1,i
      if(debug>0) print *, 'x(',j,')=', x(j), '  w(',j,')=', w(j)
      sum = sum + w(j)*exp(x(j))
    end do
    print *, i, ' integral (0.5,5.0) exp(x) dx = ', sum
  end do
  print *, 'exp(5.0)-exp(0.5) =', exp(b)-exp(a)
  print *, 'exact should be: 146.7644378'
  print *, ' '
end program gauleg
```

```
!cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
! gauleg_nr_test.f90
!
! integrates f(x)=exp(x) Gauss-Legendre
! making use of routines/modules/interfaces from Numerical Recipes in F90
! (here simplified)
!cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

program gauleg_nr_test
  use nrtype
  use nr
  implicit none
  real(sp) :: a,b,quad
  real(sp), dimension(:), allocatable :: x,w
  integer :: npts,i
  print*," insert a, b, npoints>"
  read*, a,b,npts
  allocate(x(npts))    ! allocation x and w (ascissas and weights): this
  allocate(w(npts))    ! indicates to GAULEG how many points
  call gauleg(a,b,x,w)
  do i=1,npts
     print*,x(i),w(i)
     quad=quad+exp(x(i))*w(i)
  end do
  print *,' risult=',quad,' error=',quad-(exp(b)-exp(a))
  deallocate(x,w)
  stop
end program gauleg_nr_test
```

(for the listing of `gauleg.f90` (subroutine), `nrtype.f90, nr.f90, nrutil.f90` (modules), see the full version of these exercises on the web site of the course) `gauleg.f90` from Numerical Recipes

```
SUBROUTINE gauleg(x1,x2,x,w)
  USE nrtype; USE nrutil, ONLY : arth,assert_eq,nrerror
  IMPLICIT NONE
  REAL(SP), INTENT(IN) :: x1,x2
  REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
  REAL(DP), PARAMETER :: EPS=3.0e-14_dp
  INTEGER(I4B) :: its,j,m,n
  INTEGER(I4B), PARAMETER :: MAXIT=10
  REAL(DP) :: xl,xm
  REAL(DP), DIMENSION((size(x)+1)/2) :: p1,p2,p3,pp,z,z1
  LOGICAL(LGT), DIMENSION((size(x)+1)/2) :: unfinished
  n=assert_eq(size(x),size(w),'gauleg')
  m=(n+1)/2
  xm=0.5_dp*(x2+x1)
  xl=0.5_dp*(x2-x1)
  z=cos(PI_D*(arth(1,1,m)-0.25_dp)/(n+0.5_dp))
  unfinished=.true.
  do its=1,MAXIT
     where (unfinished)
        p1=1.0
        p2=0.0
     end where
     do j=1,n
        where (unfinished)
           p3=p2
           p2=p1
           p1=((2.0_dp*j-1.0_dp)*z*p2-(j-1.0_dp)*p3)/j
        end where
     end do
     where (unfinished)
        pp=n*(z*p1-p2)/(z*z-1.0_dp)
        z1=z
        z=z1-p1/pp
        unfinished=(abs(z-z1) > EPS)
     end where
     if (.not. any(unfinished)) exit
  end do
  if (its == MAXIT+1) call nrerror('too many iterations in gauleg')
  x(1:m)=xm-xl*z
  x(n:n-m+1:-1)=xm+xl*z
  w(1:m)=2.0_dp*xl/((1.0_dp-z**2)*pp**2)
  w(n:n-m+1:-1)=w(1:m)
END SUBROUTINE gauleg
```

`nrtype.f90` from Numerical Recipes

```
MODULE nrtype
  INTEGER, PARAMETER :: I4B = SELECTED_INT_KIND(9)
  INTEGER, PARAMETER :: I2B = SELECTED_INT_KIND(4)
  INTEGER, PARAMETER :: I1B = SELECTED_INT_KIND(2)
  INTEGER, PARAMETER :: SP = KIND(1.0)
  INTEGER, PARAMETER :: DP = KIND(1.0D0)
  INTEGER, PARAMETER :: SPC = KIND((1.0,1.0))
  INTEGER, PARAMETER :: DPC = KIND((1.0D0,1.0D0))
  INTEGER, PARAMETER :: LGT = KIND(.true.)
  REAL(SP), PARAMETER :: PI=3.141592653589793238462643383279502884197_sp
  REAL(SP), PARAMETER :: PIO2=1.57079632679489661923132169163975144209858_sp
  REAL(SP), PARAMETER :: TWOPI=6.283185307179586476925286766559005768394_sp
  REAL(SP), PARAMETER :: SQRT2=1.41421356237309504880168872420969807856967_sp
  REAL(SP), PARAMETER :: EULER=0.5772156649015328606065120900824024310422_sp
  REAL(DP), PARAMETER :: PI_D=3.141592653589793238462643383279502884197_dp
  REAL(DP), PARAMETER :: PIO2_D=1.57079632679489661923132169163975144209858_dp
  REAL(DP), PARAMETER :: TWOPI_D=6.283185307179586476925286766559005768394_dp
  TYPE sprs2_sp
     INTEGER(I4B) :: n,len
     REAL(SP), DIMENSION(:), POINTER :: val
     INTEGER(I4B), DIMENSION(:), POINTER :: irow
     INTEGER(I4B), DIMENSION(:), POINTER :: jcol
  END TYPE sprs2_sp
  TYPE sprs2_dp
     INTEGER(I4B) :: n,len
     REAL(DP), DIMENSION(:), POINTER :: val
     INTEGER(I4B), DIMENSION(:), POINTER :: irow
     INTEGER(I4B), DIMENSION(:), POINTER :: jcol
  END TYPE sprs2_dp
END MODULE nrtype
```

`nr.f90` from Numerical Recipes

```
MODULE nr
  INTERFACE
     SUBROUTINE gauleg(x1,x2,x,w)
       USE nrtype
       REAL(SP), INTENT(IN) :: x1,x2
       REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
     END SUBROUTINE gauleg
  END INTERFACE
  ! ... the original file contains several other  INTERFACES ...
END MODULE nr
```

nrutil.f90 (Here only for: array_copy, arth, assert_eq, nrerror)

```
MODULE nrutil
  USE nrtype
  IMPLICIT NONE
  INTEGER(I4B), PARAMETER :: NPAR_ARTH=16,NPAR2_ARTH=8
  INTEGER(I4B), PARAMETER :: NPAR_GEOP=4,NPAR2_GEOP=2
  INTEGER(I4B), PARAMETER :: NPAR_CUMSUM=16
  INTEGER(I4B), PARAMETER :: NPAR_CUMPROD=8
  INTEGER(I4B), PARAMETER :: NPAR_POLY=8
  INTEGER(I4B), PARAMETER :: NPAR_POLYTERM=8
  INTERFACE array_copy
     MODULE PROCEDURE array_copy_r, array_copy_d, array_copy_i
  END INTERFACE
  INTERFACE assert_eq
     MODULE PROCEDURE assert_eq2,assert_eq3,assert_eq4,assert_eqn
  END INTERFACE
  INTERFACE arth
     MODULE PROCEDURE arth_r, arth_d, arth_i
  END INTERFACE
  ! ... l'originale contiene ancora molte altre INTERFACEs....
CONTAINS

  SUBROUTINE array_copy_r(src,dest,n_copied,n_not_copied)
    REAL(SP), DIMENSION(:), INTENT(IN) :: src
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
    INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
    n_copied=min(size(src),size(dest))
    n_not_copied=size(src)-n_copied
    dest(1:n_copied)=src(1:n_copied)
  END SUBROUTINE array_copy_r

  SUBROUTINE array_copy_d(src,dest,n_copied,n_not_copied)
    REAL(DP), DIMENSION(:), INTENT(IN) :: src
    REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
    INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
    n_copied=min(size(src),size(dest))
    n_not_copied=size(src)-n_copied
    dest(1:n_copied)=src(1:n_copied)
  END SUBROUTINE array_copy_d

  SUBROUTINE array_copy_i(src,dest,n_copied,n_not_copied)
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: src
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: dest
    INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
    n_copied=min(size(src),size(dest))
```

```
  n_not_copied=size(src)-n_copied
  dest(1:n_copied)=src(1:n_copied)
END SUBROUTINE array_copy_i

FUNCTION assert_eq2(n1,n2,string)
  CHARACTER(LEN=*), INTENT(IN) :: string
  INTEGER, INTENT(IN) :: n1,n2
  INTEGER :: assert_eq2
  if (n1 == n2) then
     assert_eq2=n1
  else
     write (*,*) 'nrerror: an assert_eq failed with this tag:',string
     STOP 'program terminated by assert_eq2'
  end if
END FUNCTION assert_eq2

FUNCTION assert_eq3(n1,n2,n3,string)
  CHARACTER(LEN=*), INTENT(IN) :: string
  INTEGER, INTENT(IN) :: n1,n2,n3
  INTEGER :: assert_eq3
  if (n1 == n2 .and. n2 == n3) then
     assert_eq3=n1
  else
     write (*,*) 'nrerror: an assert_eq failed with this tag:',string
     STOP 'program terminated by assert_eq3'
  end if
END FUNCTION assert_eq3

FUNCTION assert_eq4(n1,n2,n3,n4,string)
  CHARACTER(LEN=*), INTENT(IN) :: string
  INTEGER, INTENT(IN) :: n1,n2,n3,n4
  INTEGER :: assert_eq4
  if (n1 == n2 .and. n2 == n3 .and. n3 == n4) then
     assert_eq4=n1
  else
     write (*,*) 'nrerror: an assert_eq failed with this tag:',string
     STOP 'program terminated by assert_eq4'
  end if
END FUNCTION assert_eq4

FUNCTION assert_eqn(nn,string)
  CHARACTER(LEN=*), INTENT(IN) :: string
  INTEGER, DIMENSION(:), INTENT(IN) :: nn
  INTEGER :: assert_eqn
  if (all(nn(2:) == nn(1))) then
     assert_eqn=nn(1)
```

```
  else
     write (*,*) 'nrerror: an assert_eq failed with this tag:',string
     STOP 'program terminated by assert_eqn'
  end if
END FUNCTION assert_eqn

SUBROUTINE nrerror(string)
  CHARACTER(LEN=*), INTENT(IN) :: string
  write (*,*) 'nrerror: ',string
  STOP 'program terminated by nrerror'
END SUBROUTINE nrerror

FUNCTION arth_r(first,increment,n)
  REAL(SP), INTENT(IN) :: first,increment
  INTEGER(I4B), INTENT(IN) :: n
  REAL(SP), DIMENSION(n) :: arth_r
  INTEGER(I4B) :: k,k2
  REAL(SP) :: temp
  if (n > 0) arth_r(1)=first
  if (n <= NPAR_ARTH) then
     do k=2,n
        arth_r(k)=arth_r(k-1)+increment
     end do
  else
     do k=2,NPAR2_ARTH
        arth_r(k)=arth_r(k-1)+increment
     end do
     temp=increment*NPAR2_ARTH
     k=NPAR2_ARTH
     do
        if (k >= n) exit
        k2=k+k
        arth_r(k+1:min(k2,n))=temp+arth_r(1:min(k,n-k))
        temp=temp+temp
        k=k2
     end do
  end if
END FUNCTION arth_r

FUNCTION arth_d(first,increment,n)
  REAL(DP), INTENT(IN) :: first,increment
  INTEGER(I4B), INTENT(IN) :: n
  REAL(DP), DIMENSION(n) :: arth_d
  INTEGER(I4B) :: k,k2
  REAL(DP) :: temp
  if (n > 0) arth_d(1)=first
```

```
    if (n <= NPAR_ARTH) then
       do k=2,n
          arth_d(k)=arth_d(k-1)+increment
       end do
    else
       do k=2,NPAR2_ARTH
          arth_d(k)=arth_d(k-1)+increment
       end do
       temp=increment*NPAR2_ARTH
       k=NPAR2_ARTH
       do
          if (k >= n) exit
          k2=k+k
          arth_d(k+1:min(k2,n))=temp+arth_d(1:min(k,n-k))
          temp=temp+temp
          k=k2
       end do
    end if
  END FUNCTION arth_d

  FUNCTION arth_i(first,increment,n)
    INTEGER(I4B), INTENT(IN) :: first,increment,n
    INTEGER(I4B), DIMENSION(n) :: arth_i
    INTEGER(I4B) :: k,k2,temp
    if (n > 0) arth_i(1)=first
    if (n <= NPAR_ARTH) then
       do k=2,n
          arth_i(k)=arth_i(k-1)+increment
       end do
    else
       do k=2,NPAR2_ARTH
          arth_i(k)=arth_i(k-1)+increment
       end do
       temp=increment*NPAR2_ARTH
       k=NPAR2_ARTH
       do
          if (k >= n) exit
          k2=k+k
          arth_i(k+1:min(k2,n))=temp+arth_i(1:min(k,n-k))
          temp=temp+temp
          k=k2
       end do
    end if
  END FUNCTION arth_i
  !  .... and many other FUNCTIONs and SUBROUTINEs ....
END MODULE nrutil
```