بسم ا الر ن الرحيم

DEPARTMENT OF CIVIL ENGINEERING – KFUPM

Numerical and Statistical Methods in Civil Engineering

CE 318- 51- 2011-2012 (111)

Computer Lab. Sessions NO. 05 & 06

Subj.: **Using Fortran IMSL subroutine and *Mathematica* software to perform numerical inegrations**

DATE: Oct. 17,'11

Objective: mainly to perform *numerical* integration using: i) IMSL Fortran subroutine; and ii) *Mathematica* software©.

1. Use the ***Mathematica software*** to perform numerical integration of the following functions.

$f(x) = x \cos x$ for inegral limits $x_l = 1$ *and* $x_u = 4$.

Compare the *numerical results* with *exact solution* using integartion by parts formula (i.e. $\int u \, dv = vu - \int v \, du$).

2. Use the ***attached Fortarn program and subroutine*** to evaluate the integrals of the following functions using: two sampling points, three sampling points, and four sampling points for the *Gauss*-quadrature.
   Study the improvement of results and compare the errors in each case.

$$I_1 = \int_1^4 x \cos x dx$$

$$I_2 = \int_{-2}^2 \frac{dx}{1 + x^2}$$

$$I_3 = \int_0^1 x \exp(-3x^2) dx.$$

Note: In the program provided A and B are the limits of integration; NGP= the number of Gauss points; NR= number of applications of the rule of integration.

```
C     PROGRAM      REPEATED GAUSS-LEGENDRE RULE
C
C     ALTER NEXT LINE TO CHANGE PROBLEM SIZE
C
      PARAMETER (ISAMP=7)
C
      REAL SAMP(ISAMP,2)
C
      READ (5,*) A,B,NGP,NR
      CALL GAULEG(SAMP,ISAMP,NGP)
      WR = (B-A)/NR
      HR = 0.5*WR
      AREA = 0.
      DO 10 I = 1,NR
          CR = A + (I-1)*WR + HR
          DO 10 J = 1,NGP
              X = SAMP(J,1)
              W = SAMP(J,2)
              XS = CR + X*HR
   10 AREA = AREA + W*HR*F(XS)
      WRITE (6,*) ('****** REPEATED GAUSS-LEGENDRE RULE *****')
      WRITE (6,100) A,B
      WRITE (6,101) NGP
      WRITE (6,102) NR
      WRITE (6,103) AREA
  100 FORMAT (/,'  LIMITS OF INTEGRATION                 ',2F12.4)
  101 FORMAT ('  NUMBER OF GAUSS POINTS PER STRIP      ',I7)
  102 FORMAT ('  NUMBER OF REPETITIONS                 ',I7)
  103 FORMAT ('  COMPUTED RESULT                       ',F12.4)
      STOP
      END
C
      FUNCTION F(X)
C
C     THIS FUNCTION PROVIDES THE VALUE OF F(X)
C     AND WILL VARY FROM ONE PROBLEM TO THE NEXT
C
      F = write the function here!
      RETURN
      END
```

Call statement to the subroutine GAULEG

The complete Fortran file (including the Driver program, the Function, and the IntegrationSubroutine):

```
C      PROGRAM REPEATED GAUSS-LEGENDRE RULE
C      ALTER NEXT LINE TO CHANGE PROBLEM SIZE

       PARAMETER (ISAMP=7)
       REAL SAMP(ISAMP,2)
       OPEN(UNIT=5,FILE='INPUTDATA.OUT')
       OPEN(UNIT=6,FILE='OUTPUT.OUT')
       READ (5,*)A,B,NGP
       CALL GAULEG(SAMP,ISAMP,NGP)
       HR=(B-A)/2
       AREA=0
       CR=A+HR
       DO 10 J=1,NGP
       X=SAMP(J,2)
       W=SAMP(J,1)
       XS=CR+X*HR
    10 AREA=AREA+W*HR*F(XS)
       WRITE(6,*) ('***** REPEATED GAUSS-LEGENDRE RULE *****')
       WRITE(6,100)A,B
       WRITE(6,101)NGP
       WRITE(6,103)AREA
   100 FORMAT(/,'LIMITS OF INTEGRATION              ',2F12.4)
   101 FORMAT('NUMBER OF GAUSS POINTS PER STRIP   ',I7)
   103 FORMAT('COMPUTED RESULT (AREA)                  ',F12.4)
       STOP
       END
       FUNCTION F(X)
C      THIS FUNCTION PROVIDES THE VALUE OF F(X)
C      AND WILL VARY FROM ONE PROPLEM TO THE NEXT

       F=1/(1+X**2)
       RETURN
       END
       SUBROUTINE GAULEG(SAMP,ISAMP,NGP)
C      WEIGHTS AND SAMPLING POINTS
C      FOR GAUSS-LAGUERRE QUADRATURE
       REAL SAMP(ISAMP,*)
       GO TO (1,2,3,4,5),NGP
     1  SAMP(1,1)=1
       SAMP(1,2)=1
       GO TO 100
     2  SAMP(1,1)=1.0
       SAMP(2,1)=1.0
       SAMP(1,2)=-0.577350269
       SAMP(2,2)=0.577350269
       GO TO 100
    3  SAMP(1,1)=0.5555556
       SAMP(2,1)=0.8888889
       SAMP(3,1)=0.5555556
       SAMP(1,2)=-0.774596669
       SAMP(2,2)=0.0
       SAMP(3,2)=0.774596669
       GO TO 100
    4  SAMP(1,1)=0.3478548
       SAMP(2,1)=0.6521452
       SAMP(3,1)=0.6521452
       SAMP(4,1)=0.3478548
       SAMP(1,2)=-0.861136312
       SAMP(2,2)=-0.339981044
       SAMP(3,2)=0.339981044
       SAMP(4,2)=0.861136312
       GO TO 100
    5  SAMP(1,1)=0.2369269
       SAMP(2,1)=0.4786287
       SAMP(3,1)=0.5688889
       SAMP(4,1)=0.4786287
       SAMP(5,1)=0.2369269
       SAMP(1,2)=-0.906179846
       SAMP(2,2)=-0.538469310
       SAMP(3,2)=0.0
       SAMP(4,2)=0.538469310
       SAMP(5,2)=0.906179846
   100 CONTINUE
       RETURN
       END
```

Numerical Example using Mathematica:

Background on "Gauss-Legendre Quadrature:

To approximate the integral

$$\int_{-1}^{1} f[x]\, dx \approx \sum_{k=1}^{n} w_{n,k} f[x_{n,k}]$$

by *sampling* $f[x]$ at the n *unequally spaced abscissas* $x_{n,1}, x_{n,2}, \cdots, x_{n,n}$, where the corresponding weights are $w_{n,1}, w_{n,2}, \cdots, w_{n,n}$. The abscissas and weights are obtained from a table of values. The method is attributed to Johann Carl Friedrich Gauss (1777-1855) and Adrien-Marie Legendre (1752-1833).

Example 1:

Use the **Gauss-Legendre quadrature** rules for ***n* = 2, 3, and 4** points to compute numerical approximations for

$$I = \int_{-1}^{1} e^{-x^2/2}\, dx$$

Solution 1:

First, enter the formula $\text{Exp}\left[\frac{-x^2}{2}\right]$ or $E^{-x^2/2}$ or $e^{-x^2/2}$.

```
f[x_] = e^(-x^2/2);
Print["f[x] = ", f[x]];
```

$f[x] = e^{-\frac{x^2}{2}}$

Solution using Gauss-Legendre quadrature with **n = 2**:

```
w1 =  1.0 ;
w2 =  1.0 ;
x1 = -0.577350269189625 ;
x2 =  0.577350269189625 ;

Q2 = w1 f[x1] + w2 f[x2]
```

1.69296

Solution using Gauss-Legendre quadrature with **n = 3**:

```
w1 =  0.555555555555556 ;
w2 =  0.888888888888889 ;
w3 =  0.555555555555556 ;
x1 = -0.774596669241483 ;
x2 =  0.0 ;
x3 =  0.774596669241483 ;

Q3 = w1 f[x1] + w2 f[x2] + w3 f[x3]
```

1.71202

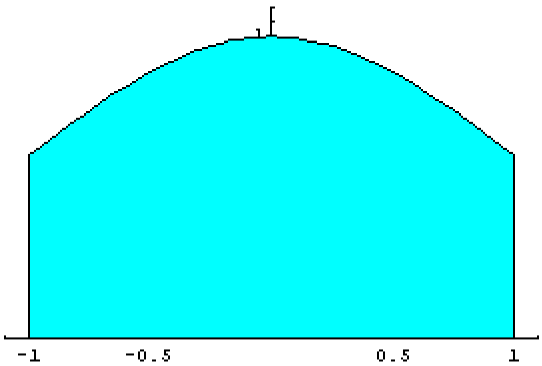
Solution using Gauss-Legendre quadrature with **n = 4**:

```
w1 =  0.347854845137453 ;
w2 =  0.652145154862546 ;
w3 =  0.652145154862546 ;
w4 =  0.347854845137453 ;
x1 = -0.861136311594053 ;
x2 = -0.339981043584856 ;
x3 =  0.339981043584856 ;
x4 =  0.861136311594053 ;

Q4 =  w1 f[x1] + w2 f[x2] + w3 f[x3] + w4 f[x4]
```

1.71122

```
line1 = Graphics[{Line[{{-1, 0}, {-1, f[-1]}}]}];
line2 = Graphics[{Line[{{1, 0}, {1, f[1]}}]}];
Needs["Graphics`Colors`"];
Needs["Graphics`FilledPlot`"];
graph = Plot[f[x], {x, -1, 1},
        PlotRange → {{-1.1, 1.1}, {0, 1.1}}];
gr1 = FilledPlot[{f[x]}, {x, -1, 1},
        Fills → {{{1, Axis}, Cyan}}];
Show[graph, gr1, line1, line2];
Print["The area under y = ", f[x]];
Print["is approximately ", Q4];
```



The area under y = $e^{-\frac{x^2}{2}}$

is approximately 1.71122

More Background [Numerical Integration [CE 318] /Extra Notes

The shifted Gauss-Legendre rule for [a,b]. To approximate the integral $\int_a^b f[t]\,dt$ use the change of variable $t = \frac{a+b}{2} + \frac{b-a}{2}x$ and $dt = \frac{b-a}{2}dx$. Then use $g[x] = f\left[\frac{a+b}{2} + \frac{b-a}{2}x\right]$ and apply the Gauss-Legendre rules for $\frac{b-a}{2}\int_{-1}^{1} g[x]\,dx$.

Exercise 3: Use the shifted Gauss-Legendre rules for n = 3 points to approximate the integrals

Illustrate the comparisons for the integral $\int_0^1 e^{-x^2/2}dx$, $\int_1^2 e^{-x^2/2}dx$ and $\int_2^3 e^{-x^2/2}dx$.

Solution. Enter the abscissas and weights. Copy them from Exercise 1 and make sure they are activated!

```
w1 =  0.555555555555556 ;
w2 =  0.888888888888889 ;
w3 =  0.555555555555556 ;
x1 = -0.774596669241483 ;
x2 =  0.0 ;
x3 =  0.774596669241483 ;
```

Exercise 3 (a: Find the integral over [0,1]

```
a = 0;
b = 1;
g[x_] = f[(a+b)/2 + (b-a)/2 x];
Q3 = (b-a)/2 (w1 g[x1] + w2 g[x2] + w3 g[x3])
```

0.855626

Compare with *Mathematica*'s calculation.

```
v1 = NIntegrate[f[x], {x, a, b}]
v1 - Q3
```

0.855624

-2.00215×10^{-6}

Exercise 3 (b): Find the integral over [1,2]

```
a = 1;
b = 2;
g[x_] = f[(a+b)/2 + (b-a)/2 x];
Q3 = (b-a)/2 (w1 g[x1] + w2 g[x2] + w3 g[x3])
```

0.34066

Compare with *Mathematica*'s calculation.

```
v2 = NIntegrate[f[x], {x, a, b}]
v2 - Q3
```

0.340664

3.40802×10^{-6}

Exercise 3 (c):

Find the integral over [2,3]

```
a = 2;
b = 3;
```

$$g[x\_] = f\left[\frac{a+b}{2} + \frac{b-a}{2}\, x\right];$$

$$Q3 = \frac{b-a}{2}\,(w1\, g[x1] + w2\, g[x2] + w3\, g[x3])$$

0.053644

Compare with *Mathematica*'s calculation.

```
v3 = NIntegrate[f[x], {x, a, b}]
v3 - Q3
```

0.0536424

-1.58428×10^{-6}

What famous numbers do you recognize in the following list ?

$$N\left[\frac{1}{\sqrt{2\pi}}\{v1, v2, v3\}\right]$$

{0.341345, 0.135905, 0.0214002}

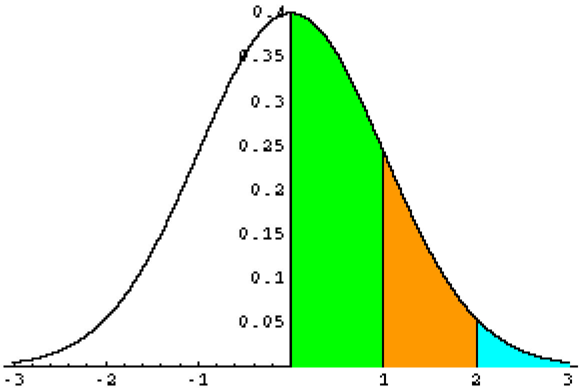
Or perhaps the following list ?

$$N\left[\frac{1}{\sqrt{2\pi}}\{v1, v2 + v1, v3 + v1 + v2\}\right]$$

{0.341345, 0.47725, 0.49865}

$$g[x\_] = \frac{1}{\sqrt{2\pi}}\, f[x];$$

```
line0 = Graphics[{Line[{{0, 0}, {0, g[0]}}]}];
line1 = Graphics[{Line[{{1, 0}, {1, g[1]}}]}];
line2 = Graphics[{Line[{{2, 0}, {2, g[2]}}]}];
gr0 = Plot[g[x], {x, -3, 0},
  PlotRange → {{-3.1, 3.1}, {0, 0.4}}];
gr1 = FilledPlot[{g[x]}, {x, 0, 1},
  Fills → {{{1, Axis}, Green}}];
gr2 = FilledPlot[{g[x]}, {x, 1, 2},
  Fills → {{{1, Axis}, Orange}}];
gr3 = FilledPlot[{g[x]}, {x, 2, 3},
  Fills → {{{1, Axis}, Cyan}}];
Show[gr0, gr1, gr2, gr3, line0, line1, line2];
```



Exercise 4: Investigate the truncation error bound formulas for the Gauss-Legendre quadrature rules of n = 2, 3, and 4 points.

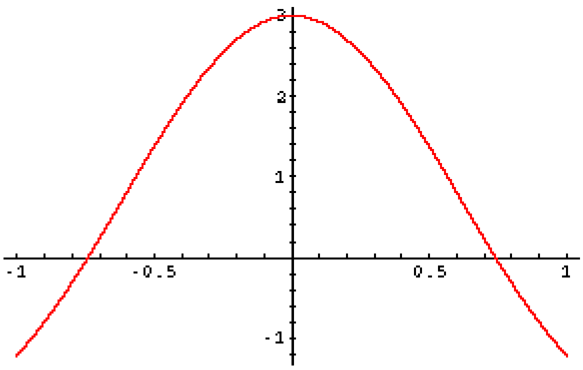
Use the integral $\int_{-1}^{1} e^{-x^2/2}\,dx$ for the investigation

Solution. Use the quadrature values obtained in Exercise 1.
Q2 = 1.692963449781228922
Q3 = 1.712020245201909760
Q4 = 1.711224504599488490

And use the "true" numerical value of the integral as found in Exercise 2
v = 1.711248783784294

Use symbolic differentiation, and a graph to determine the bound $M4 = \max_{-1 \le x \le 1} |f^{(4)}[x]|$.

```
f4[x_] = Expand[D[f[x], {x, 4}]];
M4 = Max[{Abs[f4[-1]], Abs[f4[0]], Abs[f4[1]]}];
Plot[f4[x], {x, -1, 1}, PlotStyle → Red];
Print["f''''[x] = ", f4[x]];
Print["M4 = ", M4];
```

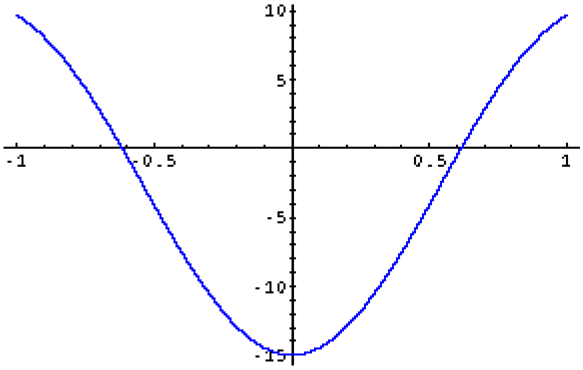


$f''''[x] = 3E^{-\frac{x^2}{2}} - 6E^{-\frac{x^2}{2}}x^2 + E^{-\frac{x^2}{2}}x^4$

M4 = 3

Use symbolic differentiation, and a graph to determine the bound $M6 = \max_{-1 \le x \le 1} |f^{(6)}[x]|$.

```
f6[x_] = Expand[D[f[x], {x, 6}]];
Plot[f6[x], {x, -1, 1}, PlotStyle → Blue];
M6 = Max[{Abs[f6[-1]], Abs[f6[0]], Abs[f6[1]]}];
Print["f''''''[x] = ", f6[x]];
Print["M6 = ", M6];
```

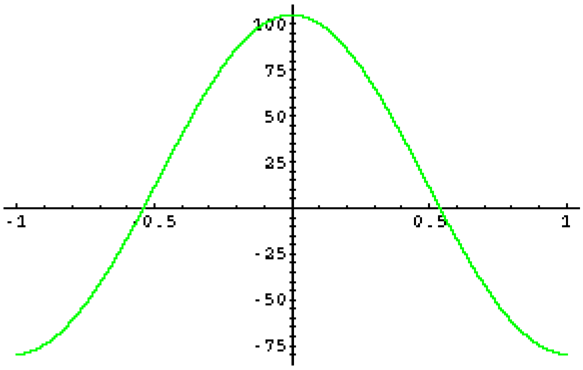


$$f''''''[x] = -15 E^{-\frac{x^2}{2}} + 45 E^{-\frac{x^2}{2}} x^2 - 15 E^{-\frac{x^2}{2}} x^4 + E^{-\frac{x^2}{2}} x^6$$

M6 = 15

Use symbolic differentiation, and a graph to determine the bound $M8 = \max_{-1 \le x \le 1} | f^{(8)}[x] |$.

```
f8[x_] = Expand[D[f[x], {x, 8}]];
Plot[f8[x], {x, -1, 1}, PlotStyle → Green];
M8 = Max[{Abs[f8[-1]], Abs[f8[0]], Abs[f8[1]]}];
Print["f''''''''[x] = ", f8[x]];
Print["M8 = ", M8];
```



$$f''''''''[x] = 105 E^{-\frac{x^2}{2}} - 420 E^{-\frac{x^2}{2}} x^2 + 210 E^{-\frac{x^2}{2}} x^4 - 28 E^{-\frac{x^2}{2}} x^6 + E^{-\frac{x^2}{2}} x^8$$

M8 = 105

Now compare the actual error and error bounds for the quadrature rules.

For n = 2, $| E_2 (f) | \le \frac{M4}{135}$.

$$EQ2 = v - Q2$$

$$EB2 = \frac{M4}{135.}$$

0.0182853

0.0222222

For n = 3, $|E_3(f)| \le \frac{M6}{15750}$.

$$EQ3 = v - Q3$$

$$EB3 = \frac{M6}{15750.}$$

-0.000771461

0.000952381

For n = 4, $|E_4(f)| \le \frac{M8}{3472875}$.

$$EQ4 = v - Q4$$

$$EB4 = \frac{M8}{3472875.}$$

0.0000242792

0.0000302343

****

Procedure for Lab.-Report Evaluation:

1. Start working in the assigned session, then complete your computer works *preferably* within the session *or* shortly afterwards using the same computing machine on which you may save your work for future use (if necessary).
2. Submit for evaluation your summary of organized computer work assignment in the beginning of the next lab.
3. Your report *should* include: i)**Introduction** expalining the work undertaken and its main objectives; ii) Clear outline of the numerical procedure(s) used; iii) **Print-out** of the work completed; and iv) **Summary** and conclusions.