UNIVERSITY OF TEXAS ARLINGTON

PHYS 5319-001:

Math Methods in Physics III

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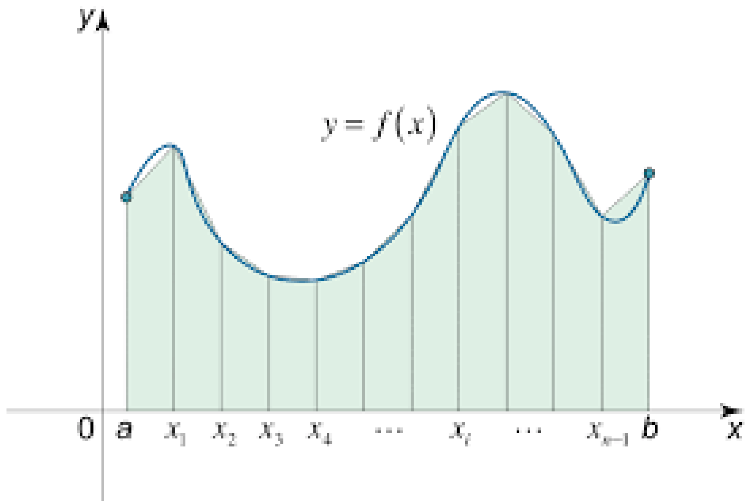
Hints of Programming

- Make a backup of your code before modifying
- Constantly save while editing
- Comments and documentation
- Use descriptive names for variables/functions
- Declare all variables (no implicit in FORTRAN: Implicit none)
- Compiler may make errors, too
- Avoid using “go to”
- Use statements (labels) as less as possible

Numerical integration

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} f(x_i)w_i$$

where **N: # of subintervals**
w_i : sum weight for *i-th* subinterval
x_i: a point in *i-th* subinterval



How to choose points/weights?

Newton-Cotes methods

$h = \frac{b-a}{N-1}$

Trapezoid rule:

$$\int_a^b f(x)dx = \frac{h}{2}f_1 + hf_2 + hf_3 + \cdots + hf_{N-1} + \frac{h}{2}f_N + O(h^2 f'')$$

Simpson rule (*N*: odd integer)

$$\int_a^b f(x)dx = \frac{h}{3}f_1 + \frac{4h}{3}f_2 + \frac{2h}{3}f_3 + \cdots + \frac{4h}{3}f_{N-1} + \frac{h}{3}f_N + O(h^4)$$

Pseudo codes

Trapezoid rule

```
SUBROUTINE TRAPZD(FUNC,A,B,S,N)
IF (N.EQ.1) THEN
  PRINT*,'NOT ENOUGH POINTS FOR TRAPEZOID'
  RETURN
ELSE
  TNM=N-1
  DEL=(B-A)/TNM  → h
  X=A+DEL
  SUM=0.
  DO J=2,N-1
    SUM=SUM+FUNC(X)
    X=X+DEL
  ENDDO
  S=0.5*(FUNX(A)+FUNC(B))+SUM
  S=S*DEL
ENDIF
RETURN
END
```

Pseudo codes

Simpson rule

```
c Simpson's rule
        subroutine simpson(f, min, max, i)
        Integer i, n
        Real*8 interval, min, max, simpson, x
        if(i.eq.1.or.mod(i,2).ne.1) then
          pring*,'odd number (>1) of points for Simpson'
          stop
        endif
        simpson=0
        interval = ((max-min) / (i-1))          h
c loop for odd points
        Do n=2, (i-1), 2
          x = interval * (n-1) + min
          simpson = simpson + 4*f(x)
        enddo
c loop for even points
        Do n=3, (i-1), 2
          x = interval * (n-1) + min
          simpson = simpson + 2*f(x)
        enddo
c add the endpoints
        simpson = simpson+f(min)+f(max)
        simpson=simpson*interval/3
        Return
        End
```

Gaussian Quadratures

non-uniform intervals

For a function $\boldsymbol{f(x)}$, $\boldsymbol{\int_a^b W(x)\, f(x) dx \approx \sum_{j=1}^{N} w_j f(x_j)}$

where $W(x)$ *is the* "weight" function in an orthogonal polynomials, don't mess with the real weight w_j

e.g. to do $\int_{-1}^{+1} \frac{\exp(-cos^2 x)}{\sqrt{1-x^2}} dx$

may choose $\boldsymbol{W(x)} = \frac{\mathbf{1}}{\sqrt{\mathbf{1-x^2}}}$ in (-1,1) window**,** called **Gaussian-Chebyshev** integration**.**

The name is usually related the corresponding orthogonal polynomials' integral weight. (recall Math-1 class)

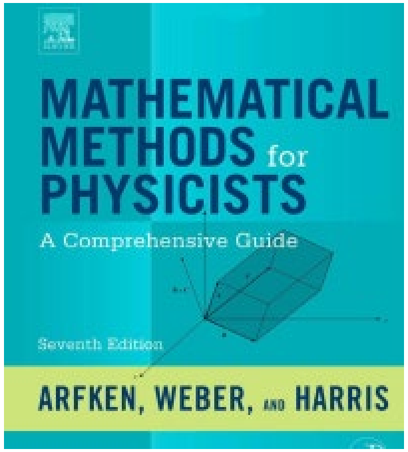


Table 5.1 Orthogonal Polynomials Generated by Gram-Schmidt Orthogonalization of $u_n(x) = x^n$, $n = 0, 1, 2, \ldots$.

Polynomials	Scalar Products	Table
Legendre	$\int_{-1}^{1} P_n(x) P_m(x) dx = 2\delta_{mn}/(2n+1)$	Table 15.1
Shifted Legendre	$\int_{0}^{1} P_n^*(x) P_m^*(x) dx = \delta_{mn}/(2n+1)$	Table 15.2
Chebyshev I	$\int_{-1}^{1} T_n(x) T_m(x) (1-x^2)^{-1/2} dx = \delta_{mn}\pi/(2-\delta_{n0})$	Table 18.4
Shifted Chebyshev I	$\int_{0}^{1} T_n^*(x) T_m^*(x) [x(1-x)]^{-1/2} dx = \delta_{mn}\pi/(2-\delta_{n0})$	Table 18.5
Chebyshev II	$\int_{-1}^{1} U_n(x) U_m(x) (1-x^2)^{1/2} dx = \delta_{mn}\pi/2$	Table 18.4
Laguerre	$\int_{0}^{\infty} L_n(x) L_m(x) e^{-x} dx = \delta_{mn}$	Table 18.2
Associated Laguerre	$\int_{0}^{\infty} L_n^k(x) L_m^k(x) e^{-x} dx = \delta_{mn}(n+k)!/n!$	Table 18.3
Hermite	$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = 2^n \delta_{mn} \pi^{1/2} n!$	Table 18.1

But, $$\int_a^b W(x)\, f(x) dx \approx \sum_{j=1}^{N} w_j f(x_j)$$ is not our usual integration form

Define $g(x) \equiv W(x) f(x)$ and $v_j \equiv w_j / W(x_j)$

The above integral becomes

$$\int_a^b g(x)\, dx \approx \sum_{j=1}^{N} v_j g(x_j) \quad \Longleftrightarrow \quad \int_a^b f(x) dx \approx \sum_{i=1}^{N} f(x_i) w_i$$

Question: How to choose abscissas/weights?

Long story but doable!

Next slide

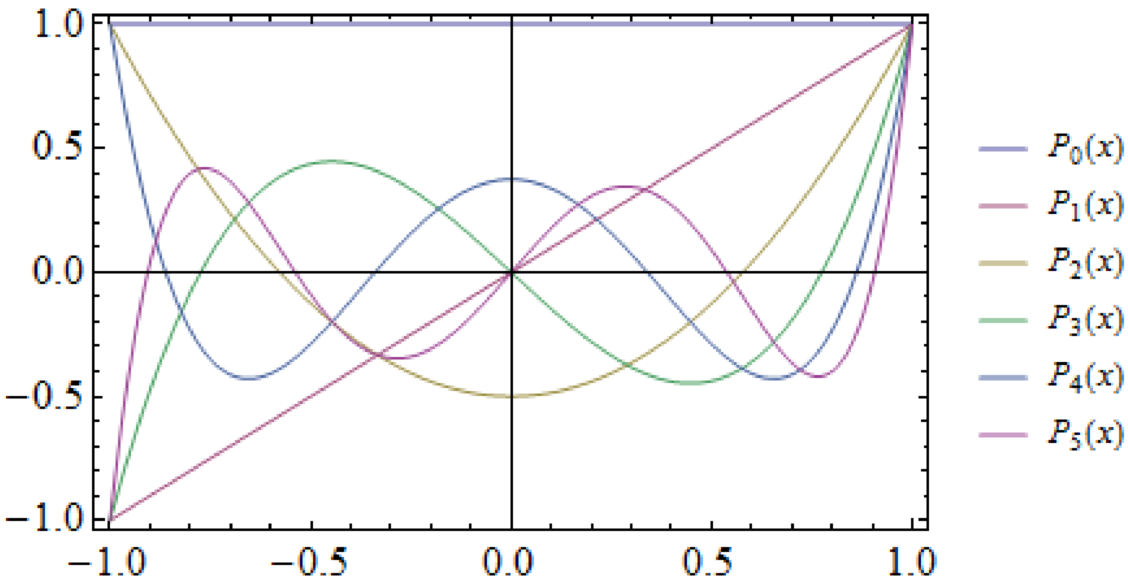
Also, accuracy?

If *f(x)* is a polynomial with the highest order less than *N*, the integration is exact.

Gaussian Quadratures (con't)

Say, the orthogonal polynomial is $p_N(x)$, *the* $\{x_j\}$ are its roots, i.e. $p_N(x_j)=0$

For example, Legendre polynomials



Due to the symmetric/antisymmetric function, only half (+) are given.

LEGENDRE POLYNOM

TABLE

$n=2$

$x_1=0.577350269189626$

$n=3$

$x_0=0.000000000000000$
$x_1=0.774596669241483$

$n=4$

$x_1=0.339981043584856$
$x_2=0.861136311594053$

$n=5$

$x_0=0.000000000000000$
$x_1=0.538469310105683$
$x_2=0.906179845938664$

$n=6$

$x_1=0.238619186083197$
$x_2=0.661209386466265$
$x_3=0.932469514203152$

$n=7$

$x_0=0.000000000000000$
$x_1=0.405845151377397$
$x_2=0.741531185599394$
$x_3=0.949107912342759$

$n=8$

$x_1=0.183434642495650$
$x_2=0.525532409916329$
$x_3=0.796666477413627$
$x_4=0.960289856497536$

$n=9$

$x_0=0.000000000000000$
$x_1=0.324253423403809$
$x_2=0.613371432700590$
$x_3=0.836031107326636$
$x_4=0.968160239507626$

$n=10$

$x_1=0.148874338981631$
$x_2=0.433395394129247$
$x_3=0.679409568299024$
$x_4=0.865063366688985$
$x_5=0.973906528517172$

Function *W(x)*

Define $\langle f|g\rangle \equiv \int_a^b W(x)f(x)g(x)dx$ $\qquad [a,b]$ *is the interval that* p_N *defined*

Gauss-Legendre:

$$W(x) = 1 \qquad -1 < x < 1$$

$$(j+1)P_{j+1} = (2j+1)xP_j - jP_{j-1}$$

Gauss-Chebyshev:

$$W(x) = (1-x^2)^{-1/2} \qquad -1 < x < 1$$

$$T_{j+1} = 2xT_j - T_{j-1}$$

Gauss-Laguerre:

$$W(x) = x^\alpha e^{-x} \qquad 0 < x < \infty$$

$$(j+1)L_{j+1}^\alpha = (-x+2j+\alpha+1)L_j^\alpha - (j+\alpha)L_{j-1}^\alpha$$

Gauss-Hermite:

$$W(x) = e^{-x^2} \qquad -\infty < x < \infty$$

$$H_{j+1} = 2xH_j - 2jH_{j-1}$$

Gauss-Jacobi:

$$W(x) = (1-x)^\alpha(1+x)^\beta \qquad -1 < x < 1$$

Weight w_i

Once the abscissas $x_1, x_2, \ldots, x_N$ are known, w_i, *i=1,2,…,N*, can be obtained

$$\begin{bmatrix} p_0(x_1) & \cdots & p_0(x_N) \\ p_1(x_1) & \cdots & p_1(x_N) \\ \vdots & & \vdots \\ p_{N-1}(x_1) & \cdots & p_{N-1}(x_N) \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{bmatrix} = \begin{bmatrix} \int_a^b W(x) p_0(x) dx \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Alternatively,

$$w_j = \frac{\langle p_{N-1} | p_{N-1} \rangle}{p_{N-1}(x_j) p'_N(x_j)}$$

where $p'_N(x_j)$ is $\frac{dp_N}{dx}$ at j-th node of $p_N(x)$.

Gauss-Legendre

$$W(x) = 1; \;\; -1 < x < 1$$

a x b

If we need to calculate $\int_a^b f(x)dx \approx \sum_{i=1}^{N} f(x_i)w_i$

-1 0 +1

x'

Rescale x to x'

$$\boldsymbol{x' = -1 + 2\frac{x-a}{b-a}}$$

Or

$$\boldsymbol{x = \frac{b-a}{2}x' + \frac{a+b}{2}}$$

The new $x' \in [-1, +1]$

Pseudo codes

Gauss-Legendre

for N = 10

```
SUBROUTINE QGAUS(FUNC,A,B,SS)
DIMENSION X(5),W(5)
DATA X/.1488743389,.4333953941,.6794095682,.8650633666,.9739065285
*/
DATA W/.2955242247,.2692667193,.2190863625,.1494513491,.0666713443
*/
XM=0.5*(B+A)
XR=0.5*(B-A)
SS=0
DO J=1,5
  DX=XR*X(J)
  SS=SS+W(J)*(FUNC(XM+DX)+FUNC(XM-DX))
ENDDO
SS=XR*SS
RETURN
END
```

Note: an arbitrary interval [A, B] is rescaled to [-1, 1] in the code!

```fortran
      SUBROUTINE GAULEG(X1,X2,X,W,N)
      REAL*4 X1,X2,X(N),W(N)
C given the lower and upper limits of the integration, X1 and X2,
C and N (n-points Gaussian), this routine returns arrays X(1:N)
C and W(1:N), the adscissas and weights of
C the Gauss-Legendre n-point quadrature formula.
      PARAMETER (EPS=3.E-14)
      M=(N+1)/2
      XM=0.5*(X2+X1)
      XL=0.5*(X2-X1)
      DO 12 I=1,M
        Z=COS(3.141592654*(I-.25)/(N+.5))
1       CONTINUE
          P1=1.D0
          P2=0.D0
          DO J=1,N
            P3=P2
            P2=P1
            P1=((2.0*J-1.0)*Z*P2-(J-1.0)*P3)/J
          ENDDO
          PP=N*(Z*P1-P2)/(Z*Z-1.0)
          Z1=Z
          Z=Z1-P1/PP
        IF(ABS(Z-Z1).GT.EPS)GO TO 1
        X(I)=XM-XL*Z
        X(N+1-I)=XM+XL*Z
        W(I)=2.0*XL/((1.0-Z*Z)*PP*PP)
        W(N+1-I)=W(I)
      ENDDO
      RETURN
      END
```

Homework-1 due next Tuesday (June 22nd)

$$V_H = \frac{1}{4\pi\varepsilon_0}\int \frac{\rho(\bar{r}')}{|\bar{r}-\bar{r}'|}\,d\bar{r}'$$

$$w_i f(\bar{r}_i)$$