***Errors***

* True Percent Relative Error:

**ε t = | true value - approximation | \* 100**

**| true value |**

* Approximate Percent Relative Error:

**ε a = | current approx. - previous approx.| \* 100**

**| current approx. |**

* Prespecified Percent Error:

**ε s = 0.5 \* 10 2 - n %** where n = desired no. of significant figures

***Numerical Methods***

***Approximation of ƒ(x)***

* ***Taylor Series Expansion:***

knowing the value of ƒ(x0) at a certain x0, ƒ(x) where x ≠ x0 can be approximated using:

**ƒ(x) = ƒ(x0) + ƒ’(x0)\*(x - x0)1  + ƒ’’(x0)\*(x - x0)2 + ... + ƒ(n) (x0)\*(x - x0)n**

**1! 2! n!**

accuracy *generally* increases as a larger n is chosen

***Approximation of a Root of a Function***

* ***Bisection Method* (Binary Search):**

**x r = x L + x U**

**2**

“sign” = sign of ƒ( x L ) \* ƒ( x U )

If sign > 0 : root is between x r and x U , so set new x L = x r and keep x U

( i.e: keep the upper bound x U )

If sign < 0 : root is between x L and x r , so keep x L and set new x U = x r

( i.e: keep the lower bound x L )

* ***False Position Method:***

**x r = x U - ƒ( x U )\*( x L - x U )**

**ƒ( x L ) - ƒ( x U )**

Similarly,

set the new values of xL and xU according to the “sign” of ƒ(xL) \* ƒ(xu)

* ***Simple Fixed Point Method:***

Requires an initial approximation “x 0”

isolate the unknown x to obtain the form:

**x i+1 = g( x i)**

In the case of *polynomials*, start by isolating the highest order term,

and then reducing it to x. (this reduces error by reducing exponents)

* ***Newton-Raphson Method* (Tangents):**

Requires an initial approximation “x0”

**x i+1 = x i - ƒ( x i)**

**ƒ'( x i)**

* ***Secant Method:***

Requires 2 initial approximations, “x0” and “x-1” (where x-1 is the value that is more towards the left of the x-axis)

**x i+1 = x i - ƒ( x i)\*( x i-1 - x i)**

**ƒ(x i-1) - ƒ(x i)**

***Approximation of a Root of a Polynomial***

* ***Müller Method:***

Requires 3 initial approximations “x0”, “x -1”, & “x -2”

**x i+1 = x i  + \_\_-2c\_\_\_\_\_\_\_\_\_**

**b ± sqrt( b2 - 4ac )**

where:

h 0 = x1 - x0

h 1 = x2 - x2

δ 0 = ƒ( x1 ) - ƒ (x0 )

h 0

δ 1 = ƒ( x2 ) - ƒ( x1 )

h 1

a = δ 1 - δ 0

h 1 + h 0

b = ah 1 + δ 1

c = ƒ( x2 )

For the denominator,

choose + or - depending on which yields a larger absolute value.

***Approximation of the Solution to a System of Linear Equations / Matrix***

* ***Gauss-Seidel Method:***

Isolate the unknowns to obtain equations of the form:

**x 1 = ( ... - ... x 2 - ... x 3 ) / ...**

**x 2 = ( ... - ... x 1 - ... x 3 ) / ...**

**x 3 = ( ... - ... x 1 - ... x 2 ) / ...**

An initial value for each unknown is required.

The most recent available value of **x i** is used in each computation;

that is:

**x 1 i + 1 = ( ... - ... x 2 i  - ... x 3 i ) / ...**

**x 2 i + 1 = ( ... - ... x 1 i + 1 - ... x 3 i ) / ...**

**x 3 i + 1 = ( ... - ... x 1 i + 1** - ... x **2 i + 1 ) / ...**

***Optimization*** *(Searching for the Minimum/Maximum Points)*

* ***Golden Search Method:***

golden ratio ≅ 0.618

given an initial range [ x L , x U ] :

**x 1 = x L + d**

**x 2 = x U - d**

where

**d = 0.618 \* ( x U - x L )**

Note that d > (0.5 \* length of range) , which means the points are in this order:

x L \_\_\_\_ x 2 \_\_\_\_\_\_\_ x 1 \_\_\_\_ x U

[\_\_\_\_\_\_\_ d \_\_\_\_\_\_\_]

To reduce the range for the next iteration (when searching for max pt. ):

**-** if **ƒ( x 1 ) > ƒ( x 2 )** , then **x 1** is optimal (closer to the max pt),

so the new range is [ **x 2 , x U** ]

- if **ƒ( x 1 ) < ƒ( x 2 )** , then **x 2** is optimal (closer to the max pt),

so the new range is [ **x L , x 1** ]

Note that the min pt. of ***ƒ(x)*** is equivalent to the max pt. of ***- ƒ(x)***

When using this method, Approximate Percent Relative Error is found by:

**ε a = 0.382 \* | ( x U - x L ) / x optimal | \* 100**

* ***Newton Method:***

Requires an initial approximation “x 0”

**x i + 1 = x i - ƒ’( x i)**

**ƒ’‘( x i)**

If **ƒ”( x ) > 0** : min pt.

If **ƒ”( x ) < 0** : max pt.

***Two-Dimensional Optimization***

given a function ƒ ( x , y ) , e.g : ƒ ( x , y ) = xy 2

and searching for an optimal point ( x , y )

* ***Hessian Matrix:***

Setting the 1st derivatives of **ƒ** to 0 returns possible min/max pts:

|d**ƒ**/dx = 0

|d**ƒ**/dy = 0

The returned point may be a minimum, maximum, or saddle point (neither).

To determine which it is, the 2nd derivative of **ƒ** must be checked:

The 2nd derivative of a many-variable function with respect to its variables

is called its Hessian. In the case of **ƒ ( x, y )** it is defined as the matrix:

**[ H ] =**  d2 **ƒ** / dx2 d2 **ƒ** / dxdy

d2 **ƒ** / dydx d2 **ƒ** / dy2

where:

d2 **ƒ** / dx2 = 2nd derivative of ƒ with respect to x

d2 **ƒ** / dy2 = 2nd derivative of ƒ with respect to y

d2 **ƒ** / dxdy = d2 **ƒ** / dydx = d( d**ƒ**/dx ) / dy = d( d**ƒ**/dy ) / dx

**Thus:**

if the determinant **|H| > 0** and **d2ƒ / dx2 > 0** : the point a **minimum**

if the determinant **|H| > 0** and **d2ƒ / dx2 < 0** : the point a **maximum**

if the determinant **|H| < 0** : the point a **saddle point** (neither)

* ***Steepest Ascent Method:***

Starting from an initial point p(x0 , y0), move in the direction of the gradient ∇ƒ

incrementally: pn+1 = pn + hn \* ∇ƒ( pn )

*i.e:*

**xn+1 = xn + hn \* ƒ ‘( xn )**

**yn+1 = yn + hn \* ƒ ‘( yn )**

To find hn :

-Replace p(x**n+1** , y**n+1**) into the multi-variable function **ƒ**

to obtain a single-variable function **g** (whose variable is **hn**)

-Derive g with respect to hn and find the root of the derivative. i.e: **g ’(hn) = 0, hn=?**

***Interpolation*** *(Approximation of Unknown Intermediate Points)*

* ***Interpolation by Lagrange Polynomial:***

Given a discrete set of data points: ( *x0* ,*ƒ(x0)* ), ( *x1* ,*ƒ(x1)* )...

approximate an unknown point p ( *x*, *ƒ(x)* ) :

**ƒn(x) = L0 ƒ(x0) + L1 ƒ(x1) + ... + Lk** **ƒ(x) + ... + Ln ƒ(xn)**

where:

Lk = (x - x0)(x - x1)...(x - xk-1)(x - xk+1) ...(x - xn) Notice: The fraction with denominator

(xk- x0)(xk- x1)...(xk- xk-1)(xk- xk+1)...(xk- xn) (x k - x k) is skipped from this product.

n

= ∏ x - xi

i=0 & i≠k xk - xi

* ***Interpolation by Newton Polynomial:***

Using this method, it is possible to make use of previous calculations as more data points are added, since ƒn(x) = ƒn-1(x) + bn(x - x0)(x - x1)...(x - xn-1)

In general,

**ƒn(x) = b0 + b1(x - x0) + b2(x - x0)(x - x1) + ... + bn(x - x0)(x - x1)...(x - xn-1)**

where,

b0 = ƒ(x0)

b1 = ƒ(x1) - ƒ(x0)

x1 - x0

ƒ(x2) - ƒ(x1) - b1

b2 = x2 - x1 *and in general:* bn = Dn-1ƒ1 - Dn-1ƒ0 = Dnƒ0

x2 - x0  xn - x0

*(where Dƒ is known as the “divided difference”)*

***Approximation of Integrals***

*xn*

*given an integral ∫ƒ(x) dx*

*x0*

*and given that the interval [x0 , xn] is divided into N segments of equal length*

*let* ***h = (xn - x0)***

***N***

*Note that h is the distance between successive abscissas x0 & x1, x1 & x2, etc.*

*ƒ(xn) is denoted as ƒn for brevity in the following*

* ***Trapezoidal Rule:***

xn

∫ƒ(x) dx = h { (ƒ0 + ƒ1) + (ƒ1 + ƒ2) + ... + (ƒn-2 + ƒn-1) + (ƒn-1 + ƒn) }

x0  2

i.e:

**xn**

**∫ƒ(x) dx = h ( ƒ0 + 2ƒ1 + 2ƒ2 + ... + 2ƒn-2 + 2ƒn-1 + ƒn)**

**x0 2**

* ***Simpson’s 1/3 Rule:***

Simpson’s rules are generally significantly more accurate than the trapezoidal rule.

Assuming n is even:

xn

∫ƒ(x)dx = h{(ƒ0 +4ƒ1 + ƒ2) + (ƒ2 +4ƒ3 + ƒ4) +...+ (ƒn-4 +4ƒn-3 + ƒn-2) + (ƒn-2 +4ƒn-1 + ƒn)}

x0 3

i.e:

xn

∫ƒ(x)dx = h (ƒ0 + 4ƒ1 + 2ƒ2 + 4ƒ3 + 2ƒ4 +...+ 2ƒn-4 + 4ƒn-3 + 2ƒn-2 + 4ƒn-1 + ƒn)

x0 3

i.e:

**xn**

**∫ƒ(x)dx = h ( ƒ0 + 4∑ƒodd-numbers + 2∑ƒeven-numbers + ƒn )**

**x0 3**

* ***Simpson’s 3/8 Rule:***

Has a fixed formula; fixed at N = 3 and n = 3:

**h = x3 - x0**

**3**

**x3**

**∫ƒ(x)dx = 3h ( ƒ0 + 3ƒ1 + 3ƒ2 + ƒ3 )**

**x0 8**

* ***2-Point Gauss-Legendre:***

The interval of the integral must be [-1,1 ]

If it is not, any definite integral can be changed to an integral over [-1,1 ] using a variable substitution known as Gauss-Legendre translation:

**xnew = (xn - x0) xold + (xn + x0)**

**2 2**

**dxnew = (xn - x0) dxold**

**2**

i.e: xn 1 1

∫ƒ(x) dx = (xn - x0) ∫ƒ( (xn - x0) x + (xn + x0) ) dx = ∫ƒ(xnew) dxnew

x0 2 -1 2 2 -1

The 2-Point Gauss Legendre formula can now be applied:

**1**

**∫ƒ(x) dx = f( -1 ) + f( 1 )**

**-1 ( √3 ) ( √3 )**

This approximation formula actually gives the exact result for polynomials of degree ≤ 3

***Approximation of Solutions of Ordinary Differential Equations***

*given y'(t) = ƒ(t, y) (i.e. ƒ denotes the 1st derivative) and y(t0) = y0*

*as well as a step size* ***h****, where h is also the difference between successive tn-1 & tn*

* ***Euler’s Method:***

Low accuracy

**yn+1 = yn + hƒ(tn, yn)**

* ***Midpoint Method:***

High accuracy

**yn+1 = yn + k2 h**

where:

**k1 = ƒ(xn, yn)**

**k2 = ƒ(xn + h , yn + k1 h )**

**2** **2**

* ***Runge-Kutta Method:***

Less accurate than Midpoint Method

**yn+1 = yn + ( k1 + k2 )h**

**2 2**

where:

**k1 = ƒ(xn, yn)**

**k2 = ƒ(xn + h , yn + k1 h )**