Computer Simulations

A practical approach to simulation

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Basics of Numerical Analysis

Taylor Series Expansion

- In this chapter we will discuss the main ideas of numerical computations and computational science by taking a very simple approach, namely only considering Taylor series expansion of a function.

Basics of Numerical Analysis

Taylor Series Expansion

- When a continuous function is represented on a discrete space-mesh, the smallest difference can not be less than the difference between two points on the mesh.
- Function has discrete values on the mesh. Never the less continuous function values can be obtained between these discrete points. Starting at the i^{th} point of the mesh whose coordinate is x_i, the value of the function at any point between two points i and $i+1$ can be obtained by considering the Taylor's series expansion (as apolynom) of the function.

Basics of Numerical Analysis

Taylor Series Expansion

- $$\begin{aligned} f(x_i + \Delta x) = f(x_i) + \left.\frac{df}{dx}\right|_{x=x_i} \Delta x &+ \frac{1}{2!} \left.\frac{d^2 f}{dx^2}\right|_{x=x_i} \Delta x^2 \\ &+ \frac{1}{3!} \left.\frac{d^3 f}{dx^3}\right|_{x=x_i} \Delta x^3 + \cdots \end{aligned}$$

- Expanding a function into Taylor series and taking a certain number of terms in this series corresponds to approximating the function by a polynomial.

Basics of Numerical Analysis

Taylor Series Expansion

- The essence of numerical computation lies in expanding a function to a polynomial and doing calculations analytically in valid and controllable fashion in a small interval. Summing all these small intervals give the desired solution in the actual interval.

Basics of Numerical Analysis

Difference Derivatives in Space

- Function values are defined on the mesh points, $i, \quad i = 0 \cdots N$. By taking Δx as the distance between the mesh points $\Delta x = x_{i+1} - x_i$.
- Difference derivative can be obtained in discrete form using Taylor series expansion:

$$f(x_i + \Delta x) = f(x_i) + \left.\frac{df}{dx}\right|_{x=x_i} \Delta x + \mathcal{O}(\Delta x^2)$$

- By rearranging the expansion, Eq.(6),

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} + \mathcal{O}(\Delta x)$$

Basics of Numerical Analysis

Difference Derivatives in Space

- $$\frac{\Delta f}{\Delta x} = \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

  This form of the approximate first derivative is called 2-Point Forward difference formula since the difference is considered with a forward point.

- Similarly, from expansion of $f(x_i - \Delta x)$ 2-Point backward difference derivative formula can be obtained.

  $$\frac{\Delta f}{\Delta x} = \frac{f(x) - f(x-\Delta x)}{\Delta x}$$

Basics of Numerical Analysis

Difference Derivatives in Space

- Forward and backward difference formulas are good approximations to the first derivative df/dx if $f(x)$ does not change very rapidly over Δx.
- In this approximation the error is of the order of Δx.
- In order to increase the accuracy, difference between the mesh points must be decreased in other word the existing interval $x_{i+1} - x_i$ must be divided into smaller intervals.

Basics of Numerical Analysis

Difference Derivatives in Space

- When it is possible to reduce Δx, one may run into another type of difficulty:
- If the function f is a very smooth function, i.e., the change in the function in this interval is less than the machine accuracy, the discrete derivative of the function may be unpredictable.
- Hence reducing Δx is not a solution.
- In some cases the function values are provided at discrete points.
- In this case it is not possible to reduce the distance between the mesh points.

Basics of Numerical Analysis

Difference Derivatives in Space

- New more accurate approximations must be found.
- More accurate approximations can be obtained by including more terms in the Taylor series expansion.
- Method of obtaining more accurate formula is to cancel higher terms in the Taylor series.
- Expand the function at various mesh points and combine them in such a way that only very high order terms in the expansion will remain.

Basics of Numerical Analysis

Difference Derivatives in Space

- A three point formula can be written by using Taylor expansion of the function f at the mesh points x_{i+1} and x_{i-1}.

$$f(x_i+\Delta x) = f(x_i)+\left.\frac{df}{dx}\right|_{x=x_i}\Delta x+\frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x=x_i}\Delta x^2+\mathcal{O}(\Delta x^3)$$

$$f(x_i-\Delta x) = f(x_i)-\left.\frac{df}{dx}\right|_{x=x_i}\Delta x+\frac{1}{2}\left.\frac{d^2 f}{dx^2}\right|_{x=x_i}\Delta x^2-\mathcal{O}(\Delta x^3)$$

Basics of Numerical Analysis

Difference Derivatives in Space

- Substracting these formulas, a first derivative formula is obtained with $\mathcal{O}(\Delta x^2)$ accuracy.

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_i + \Delta x) - f(x_i - \Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

Basics of Numerical Analysis

Difference Derivatives in Space

- First derivative:

```
/*----------------------------------------------------
double Deriv_1(double func(double x),double x0 ,
{return(((func(x0+dx)-func(x0-dx))/(2*dx)));}
/*----------------------------------------------------
```

- Second derivative:

```
/*----------------------------------------------------
double Deriv_2(double func(double x),double x0,c
{return(((func(x0+dx)+func(x0-dx)-2.0*func(x0))/
/*------- -------------------------------------------
```

Basics of Numerical Analysis

Difference Derivatives in Space

- Similarly the accuracy can be increased further by expanding the function at five different mesh points, $x_{i-2}, x_{i-1}, x_{i+1}, x_{i+2}$.

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{1}{8\Delta x}(f(x_i - 2\Delta x) - 8f(x_i - \Delta x) + 8f(x_i + \Delta x)$$
$$+f(x_i + 2\Delta x)) + \mathcal{O}(\Delta x^4)$$

Basics of Numerical Analysis

Difference Derivatives in Space

- Second and higher order derivatives can be obtained analogously.
- Second order derivative of a function f can be simply written from the summing taylor series expansions of $f(x_i + \Delta x)$ and $f(x_i + \Delta x)$.

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x_i} = \frac{f(x_i + \Delta x) - 2f(x_i) + f(x_i - \Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^4)$$

- This formula can also be obtained by applying first derivative twice on the function, $\frac{d^2 f(x)}{dx^2} = \frac{d(f(x+\Delta x) - f(x))/\Delta x}{dx}$.

Basics of Numerical Analysis

Difference Derivatives in Space

- More accurate the second derivative formula can be obtained by considering Taylor series expansion of the function $f(x)$ at five different mesh points, $x_{i-2},\ x_{i-1},\ x_{i+1},\ x_{i+2}$.
-

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x_i} = \frac{1}{12\Delta x^2}(-f(x_i-2\Delta x)-16f(x_i-\Delta x)-30f(x_i) +16f(x_i+\Delta x)-f(x_i+2\Delta x))+\mathcal{O}(\Delta x^4)$$

Basics of Numerical Analysis

Partial derivatives:

- Partial derivatives can olso be obtained by using difference derivatives:

$$
\begin{aligned}
f(x+\Delta x, y) &= f(x,y) + \frac{\partial f}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}\Delta x^2 + \mathcal{O}(\Delta x^3) \\
f(x, y+\Delta y) &= f(x,y) + \frac{\partial f}{\partial y}\Delta y + \frac{1}{2}\frac{\partial^2 f}{\partial y^2}\Delta y^2 + \mathcal{O}(\Delta y^3) \\
f(x+\Delta x, y+\Delta y) &= f(x,y) + \frac{\partial f}{\partial x}\Delta x + \frac{\partial f}{\partial y}\Delta y + \frac{1}{2}(\frac{\partial^2 f}{\partial x^2}\Delta x^2 + \\
&\quad \frac{\partial^2 f}{\partial y^2}\Delta y^2) + \frac{\partial^2 f}{\partial x \partial y}\Delta x \Delta y + \mathcal{O}(\Delta^3)
\end{aligned}
$$

Basics of Numerical Analysis

Partial derivatives:

- Partial derivatives with respect to x and y in terms of difference derivatives:

$$\frac{\partial f(x,y)}{\partial x} = \frac{f(x+\Delta x, y) - f(x,y)}{\Delta x}$$

$$\frac{\partial f(x,y)}{\partial y} = \frac{f(x, y+\Delta y) - f(x,y)}{\Delta y}$$

Basics of Numerical Analysis

Interpolation

- In many problems of function values may be obtained in discrete points.
- Two most common examples of discrete function values are:
  - The experimental values of an observable.
  - Tabulated values of some functions.
- In either case commonly a value between the given points may be necessary.
- At this point interpolation come into play.

Basics of Numerical Analysis

Interpolation

- In numerical analysis there are many methods of interpolation in order to meet the special requirement of the problem.
- In some cases known points are equally spaced and in some other case the independent variable may be chosen arbitrarily.
- Here in this section the aim is to give the feeling of interpolation rather than to give an explicit account of this method.
- For this aim, the discrete Taylor series expansion of the function at the point x_i is sufficient.

Basics of Numerical Analysis

Interpolation

- Calculate the value of $f(x)$, $x_i < x < x_{i+1}$.

$$f(x) \;=\; f(x_i) + \left.\frac{df}{dx}\right|_{x=x_i} \Delta x + \frac{1}{2}\left.\frac{d^2 f}{dx^2}\right|_{x=x_i} \Delta x^2 + \mathcal{O}(\Delta x^3)$$

- As a first approximation the first derivative may be replaced by difference formula,

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{\Delta x}$$

Considering only the terms up to second order, Taylor series become,

$$f(x) \;=\; f(x_i) + \frac{f(x_{i+1}) - f(x_i)}{\Delta x}(x - x_i)$$

Basics of Numerical Analysis

Interpolation

- will lead to,

$$f(x) \;=\; [1-\varepsilon]f(x_i) + \varepsilon f(x_{i+1})$$

  where $\varepsilon = \frac{x-x_i}{x_{i+1}-x_i}$.

- If $f(x)$ is a smooth function in the considered interval, this approximation is a reasonable representation of the function $f(x)$ at the point x which lies in between the mesh points x_i and x_{i+1}.
- For better approximation, higher order polynomials will be necessary.

Basics of Numerical Analysis

Interpolation

- Calculating the function at three points, one can obtain a better approximation: a quadratic polinom.
- By using difference formulas,the Taylor seies expansion around x_i is,

$$
\begin{aligned}
f(x) &= f(x_i) + \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x}(x - x_i) + \\
&\quad \frac{1}{2}\frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{\Delta x^2}(x - x_i)^2 \\
&\quad + \mathcal{O}(\Delta x^3) \qquad (1)
\end{aligned}
$$

where only the terms up to $\mathcal{O}(\Delta x^3)$ is considered.

Basics of Numerical Analysis

EXAMPLES

1. Tabulated values of $sin\theta$ are:

θ	$\sin\theta$
0.80	0.71736
0.81	0.72429
0.82	0.73115

   Obtain values in between the tabulated values.
   Check:Use $x_1 = 0.80,\ x_2 = 0.82$ and obtain
   $x = 0.81\ \ f = 0.72426$ is reasonable.
2. Given a set of data points check which ones are out of place.

Basics of Numerical Analysis

Roots of a Function

- Finding the roots of a function is one of the most commonly met problems of numerical analysis.
- By definition, a is a root of f, if $f(a) = 0$.
- However in numerical applications it must be understood that the equation usually can not be satisfied exactly due to round-off errors and limited capacity.
- Therefore the mathematical definition of a root must be modified.

Basics of Numerical Analysis

Roots of a Function

- The condition of having a root at $x = a$ may be modified such that $|f(a) < \epsilon|$, where ϵ is a given tolerance suffices.
- The inequality defines an interval instead of a point. Assuming the function value is known at a point x_o which is at the vicinity of the root of the function.

Basics of Numerical Analysis

Roots of a Function

- Taylor series expansion, at $x = x_o + \Delta x$:

$$f(x) = f(x_0) + \left.\frac{df}{dx}\right|_{x=x_0} \Delta x + \mathcal{O}(\Delta x^2)$$

- $f(x)$ will be equal to zero if $x_o + \Delta x$ is the unknown root of the function.
- Hence root of the function can be obtained as,

$$f(x_0) + \left.\frac{df}{dx}\right|_{x=x_0} (x - x_0) = 0, \quad \longrightarrow \quad x = x_0 - \frac{f(x_0)}{\left.\frac{df}{dx}\right|_{x=x_0}}$$

Basics of Numerical Analysis

Roots of a Function

- This formula is known as Newton-Rapson formula.
- In fact, it is not possible to know a point x_o that is very close to the actual root of the function.
- This method is used to generate a sequence of values x^i, converging to true root value x.
- $$x_{i+1} = x_i - \frac{f(x_i)}{df(x)/dx|_{x_i}}$$

Basics of Numerical Analysis

Roots of a Function

- Newton-Rapson root-finding program

```
/*------------------------------------------
double Newton(double f(double x),double deriv(do
{#define MAXCOUNT 100
double x,xn,count=0;
xn = x0;
 do{ x = xn;
     xn = x - (f(x)/deriv(x));
     count++;
  }while((fabs(xn-x) >= acc) && ( count < MAXCOU
return(xn);}
/*------------------------------------------
```

Basics of Numerical Analysis

Roots of a Function

- The difficulty with the Newton-Rapson formula is the requirement of the derivative of the function.
- This difficulty is eased if the derivative at point x_i is replaced with the difference formula,

$$fracdf(x)dx\Big|_{x_i} \simeq \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

- The Newton-Rapson formula then becomes,

$$x_{i+1} = x_i - f(x_i)\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}$$

which is called Secant formula.

Basics of Numerical Analysis

Roots of a Function

- Secant algorithm:

```
/*-----------------------------------------------
double Secant(double f(double x),double x0,doubl
{#define MAXCOUNT 100
double x,xn,deltax=0.001,count=0;
xn = x0;
do{ x = xn;
    xn = x - (2*deltax*f(x)/(f((x+deltax))-f((x-
  }while((fabs(xn-x) >= acc) && ( count++ < MAXC
return(xn);
}
/*-----------------------------------------------
```

Basics of Numerical Analysis

Roots of a Function

- It can be shown that the convergence of the Newton-Rapson/Secant method is quadratic.
- This fact also means that the number of correct decimals is approximately doubled at every iteration at least if the factor $f''(a)/2f'(a)$ is not too large.
- The method can be used both algebraic and transcendental equations, and it also works when coefficients of roots complex.

Basics of Numerical Analysis

Roots of a Function

- The derivation presented here assumes that the desired root is simple.
- If the root is of multiplicity $P > 1$ the convergence speed is given by $\epsilon_{n+1} \simeq [(P-1)/P]\,\epsilon_n$
- The modified formula,

$$x_{n+1} = x_n - \frac{pf(x_n)}{f'(x_n)}$$

restores the quadratic convergence.

Basics of Numerical Analysis

Roots of a Function

- If the multiplicity is not known we can instead search for a zero of this function $f(x)/f'(x)$.
- Assuming that $f'(x)$ finite everywhere this function has the same zeros as $f(x)$ with only difference that all zeros are simple.
- This leads to the formula

$$x_{n+1} = x_n - \frac{f(x_n)f'(x_n)}{f'^2(x_n) - f(x_n)f''(x_n)}$$

where again quadratic convergence is restored.

Basics of Numerical Analysis

Roots of a Function

- Despite the speedy convergence of the method, convergence depends on the initial value.
- If the initial value is not chosen near the root, either convergence is very slow or even divergence from the root is possible.
- Before starting the Newton-Rapson routine it is generally advisable to locate the roots of the function by using a crude method.

Basics of Numerical Analysis

Roots of a Function

- In some suitable method construct a sequence of numbers,$x_1, x_2, x_3, \ldots, x_n$ where $x_1 < x_2 < x_3 < \ldots < x_n$.
- If $f(x_n)f(x_n + 1) < 0$, at least a root must lie in between the points x_n and x_{n+1},in which case $x_0 = \frac{1}{2}(x_n + x_{n+1})$ is a good starting value for Newton-Rapson or secant method.

Basics of Numerical Analysis

Roots of a Function

- Bisection Algorithm:

```
double Bisect(double fnct(double x),double a,dou
{
double x0=0.0,x1=(a<b?a:b),x2 =(a<b?b:a),deltax
f1 = fnct(x1);f2 = fnct(x2);
  do {if(f1 * f2 < 0)
         { deltax = deltax / 2.0;  x0 = x1 + del
     if(f0 * f1 < 0.0 )f2 = f0;  else { x1 = x0;
          }
  }while((deltax > eps) && (*ierr == 0));
return(x0);
}
```

Basics of Numerical Analysis

Roots of a Function

- Roots of a complex function:
- It should be noted that in the case of an algebraic equation with real coefficients, a complex root can not be reached with a real starting value.
- For the complex case Newton-Rapson formula becomes,

$$Z_{n+1} = Z_n - \frac{f(z)}{f'(z)}$$

.

Basics of Numerical Analysis

Roots of a Function

- $$x^4 - x = 10$$

  By Newton-Rapson formula, setting $f(x) = x^4 - x - 10$ we get

$$\begin{aligned} x_{n+1} &= x_n - \frac{x_n^4 - x_n - 10}{4x_n^3 - 1} = \frac{3x_n^4 + 10}{4x_n^3 - 1} \\ x_0 &= 2 \\ x_1 &= 1.871 \\ x_2 &= 1.85578 \\ x_3 &= 1.855585 \end{aligned}$$

(2)

Basics of Numerical Analysis

Roots of a Function

- Find the square root of a number.

$$\sqrt{a} = x$$

or

$$f(x) = x^2 - a$$

Then in Newton-Rapson method,

$$x_{n+1} = x_n - \frac{x_n^2 - a}{2x_n}$$

a=2	a=2	a=7
$x_0 = 2$	$x_0 = 5$	$x_0 = 1$
$x_1 = 1.5$	$x_1 = 2.7$	$x_1 = 4$
$x_2 = 1.41666$	$x_2 = 1.720$	$x_2 = 2.875$

Basics of Numerical Analysis

Roots of a Function

- Find the roots of the function,

$$f(x) = x^3 - x$$

by using Nweton-Rapson method.

$$f'(x) = 3x - 1$$

$$x_{n+1} = x_n - \frac{x_n^3 - x_n}{3x_n - 1}$$

Roots are, $x = 0,\ x = 1\ and\ x = -1$ choose $x_0 = -0.4472,\ -0.44725\ and\ -0.4473$ to which root it converges?

Basics of Numerical Analysis

Integration

- In this section we are interested in calculating definite integral of a continuous function $f(x)$ between two limits, $a - b$ $(a < b)$.
- In numerical integration function may be known at some discrete values, x_i, of the independent variable x.
- Knowing a vector of function values (f_i), if a good interpolation can give the function value at any point in the interval Δx, between the known values of the function, the integral becomes a success.

Basics of Numerical Analysis

Integration

- Hence for integration, interpolation plays the most important role.
- An interpolation method can be used to obtain the function as a polinomial in the interval x_i and x_{i+1}.
- Analitical integration of the polinomial is the approximate numerical integral of this function in this interval.
- Summing all intervals between the end points,a and b give the desired integral.
- The error on the integration is also closely dependent on the error of representing the function between the mesh points.

Basics of Numerical Analysis

Integration

- There are many integration algorithms based on different levels of sophistication.
- Here, we will discuss one of the methods which is based on Taylor series expansion up to $\mathcal{O}(\Delta x^3)$, namely Simpson integration algorithm.
- For Simpson's integration algorithm equally spaced even number of intervals are considered: $N(even)$.
- N Function values will be calculated,

$$N = \frac{b-a}{\Delta x}$$

Basics of Numerical Analysis

Integration

- Since the integral may be written as the sum of integrals it is sufficient to define an interpolation formula for the interval $2\Delta x$.

$$\int_a^b f(x)dx = \int_a^{a+2\Delta x} f(x)dx + \int_{a+2\Delta x}^{a+4\Delta x} f(x)dx + \ldots + \int_{b-2\Delta x}^{b} f(x)dx$$

Basics of Numerical Analysis

Integration

- If the function is a smooth function, in these small intervals a Taylor series expansion at the middle of the interval may be a good approximation. By making appropriate change of variable integrals over the interval of $2\Delta x$ may be written such that,

$$\int_{x_0-\Delta x}^{x_0+\Delta x} f(x)dx$$

Basics of Numerical Analysis

Integration

- By using difference formulas,the Taylor seies expansion at x_o is,

$$
\begin{aligned}
f(x) &= f(x_0) + \frac{f(x_0+\Delta x) - f(x_0-\Delta x)}{2\Delta x}(x-x_0) + \\
& \frac{1}{2}\frac{f(x_0+\Delta x) - 2f(x_0) + f(x_0-\Delta x)}{\Delta x^2}(x-x_0)^2 \\
& +\mathcal{O}(\Delta x^3) \qquad (3)
\end{aligned}
$$

where only the terms up to $\mathcal{O}(\Delta x^3)$ is considered.

Basics of Numerical Analysis

Integration

- since the interval is symmetric, no contribution comes from the odd terms. Considering all terms up to the order Δx^3,

$$\int_{x_0-\Delta x}^{x_0+\Delta x} f(x)dx = \frac{\Delta x}{3}(f(x_0-\Delta x)+4f(x_0)+f(x_0+\Delta x))+\mathcal{O}(\Delta x^5)$$

  here since $\mathcal{O}(\Delta x^3)$ term has no contribution, the error term is at $\mathcal{O}(\Delta x^5)$.

Basics of Numerical Analysis

Integration Examples

- This formula is known to be Simpson's rule. Summing up all terms from a to b, the integral becomes,

$$
\begin{aligned}
\int_a^b f(x)dx \quad = \quad & \frac{\Delta x}{3}[f(a) + 4f(a+\Delta x) + 2f(a+2\Delta x) \\
& +4f(a+3\Delta x) + 2f(a+4\Delta x) + \ldots \\
& +2f(b-2\Delta x) + 4f(b-\Delta x) + f(b)]
\end{aligned}
$$

Basics of Numerical Analysis

Integration Examples

- Simpson integration algorithm:

```
/*-------------------------------------------------
double Simpson(double func(double x), double a,
{double x = a, delx = (b - a)/(2.0*n),sum1=0.0,s
int i;
for(i=1;i<=n;i++)
     {
        x += delx; sum1 += func(x);
        x += delx; sum2 += func(x);
     }
return(delx*(func(a)+4*sum1+2*sum2-func(b))/3.0)
}
/*-------------------------------------------------
```

Basics of Numerical Analysis

Integration Examples

- Take the integral of $f(x) = x^3$ by using both Simpson's rule for $N = 2, 10, 100$.
- Compare the results. For small number of intervals $N = 2, 4 \ldots$
- Hint: For $N = 2, 4 \ldots$, one can do the calculations by hand.

Basics of Numerical Analysis

Integration

Examples

- By taking only the first term of the series expansion, the integral in a small interval $x_0 - \Delta x < x < x_0 + \Delta x$ becomes,

$$\int_{x_0-\Delta x}^{x_0+\Delta x} f(x)dx = 2\Delta x f(x_0) + \mathcal{O}(\Delta x^3)$$

and hence full integral is:

$$\int_a^b f(x)dx = 2\Delta x[f(a) + f(b) + \sum_{i=1}^{N/2-1} f(x_{2i})]$$

Take the integral of $f(x) = x^3$ by using both Simpson's rule and above simplified approximation. Compare the

Basics of Numerical Analysis

Integration Examples

- To calculate an integral,

$$\int_a^b f(x)dx = \sum_{i=0}^{N-1} \int_{a+i\times\Delta x}^{a+(i+1)\times\Delta x} f(x)dx$$

expand the function into Taylor's series, and take one, two three . . . terms to obtain new integration formulas. No restriction on the number of intervals.

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- Many of the processes are most conveniently formulated in terms of differential equations.
- An ordinary differential equation is an equation containing one independent and one dependent variable.
- At least one derivative of the dependent variable with respect to independent variable must exist.
- Non of the two variable need enter the equation explicitly.
- If the equation is of such a form that the highest (n^{th}) derivative determine the order of the differential equation.

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- the highest (n^{th}) derivative can be expressed as a function of lower derivatives and dependend and independent variables.
- It is possible to replace the equation by a system of n first order equations by use of simple substitution techniques.

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- One of the most commonly met example is equation of motion,

$$\frac{d^2x}{dt^2} = \frac{1}{m}F(x, \dot{x}, t)$$

- which can easily be written as two coupled first order differential equations:

$$\begin{aligned} \frac{dx}{dt} &= v \\ \frac{dv}{dt} &= \frac{1}{m}F(x, v, t) \end{aligned}$$

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- In some cases the system in consideration can be explained in terms of coupled first order differential equations.

$$
\begin{aligned}
\frac{dx_1}{dt} &= F_1(x_1, x_2, \ldots, x_N, t) \\
\frac{dx_2}{dt} &= F_2(x_1, x_2, \ldots, x_N, t) \\
\frac{dx_3}{dt} &= F_3(x_1, x_2, \ldots, x_N, t) \\
\vdots \frac{dx_N}{dt} &= F_N(x_1, x_2, \ldots, x_N, t)
\end{aligned} \tag{4}
$$

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- Hence the discussion of higher order differential equations or coupled system of differential equations can be reduced to the solution of first order differential equations.
- Without loss of generality examination of the equation,

$$y' = f(x, y)$$

  give answer to the problem of solutions of higher order differential equations or systems of differential equations.

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- The simplest possible solution to the first order differential equation may be that the derivative of the dependent variable is replaced by difference equation,

$$y_{n+1} = y_n + \Delta x \; f(x_n, y_n)$$

- This method is called Euler's first order method.
- its accuracy is closely dependent on the choice of Δx.
- The error is governed by the error of difference approximation ($\mathcal{O}(\Delta x)$).

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

Euler algorithm

```
/*-------------------------------------------------------
double Euler(double f(double x, double y, double z)
double x,double y,double dx)
{
/*---------------------  ---------------------------
    This program uses the Euler method to solve
    dy/dx = f(x,y(x))
    y_n+1 = y_n + f(x_n,y_n)*dx    Error is O(h^2)
------------------------------------------------------*/
  return( y + f(x,y)*dx);
}/*End of function Euler */
/*-----------------------------------------------------*
```

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- Methods of higher accuracy may be derived but at a price of calculating function value at many different points.

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- Runge-Kutta integration of first order diff. equations

$$
\begin{aligned}
y_{n+1} &= y_n + \Delta x f(x_{n+\Delta x/2}, y_{n+1/2}) \\
y_{n+1} &= y_n + \Delta x [f(x_n, y_n) + \frac{\Delta x}{2}\frac{df(x_n, y_n)}{dx} + \mathcal{O}(\Delta x^2)] \\
y_{n+1} &\simeq y_n + \Delta x f(x_n, y_n) + \frac{\Delta x^2}{2}\frac{df(x_n, y_n)}{dx}
\end{aligned}
$$

Basics of Numerical Analysis

Integration of Ordinary Differentiate Equations

- Forth order Runge-Kutta integration of first order diff. equations

$$
\begin{aligned}
k_1 &= \Delta x f(x_{n+}, y_n) \\
k_2 &= \Delta x f\left(x_n + \frac{\Delta x}{2}, y_n + \frac{k_1}{2}\right) \\
k_3 &= \Delta x f\left(x_n + \frac{\Delta x}{2}, y_n + \frac{k_2}{2}\right) \\
k_4 &= \Delta x f(x_n + \Delta x, y_n + k3) \\
y_{n+1} &= y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}
$$

Basics of Numerical Analysis

```
double RungeKutta(double f(double x, double y), \
double x,double y,double h){
/*---------------------------------------------------
     Forth order Runge-Kutta method to solve
        dy/dx = f(x,y(x))  Error is O(h^5)
---------------------------------------------------
  double k1,k2,k3,k4,h2;
  h2 = 0.5 * h;
  k1 = f(x,y);  x += h2;
  k2 = f(x,y+k1*h2); k3 = f(x,y+k2*h2);
  x += h2;  k4 = f(x,y+k3*h);
  return(y+h*(k1+2*(k2+k3)+k4)/6.0L);
}/*End of function Runge-Kutta */
```

Basics of Numerical Analysis

If $f(x, y)$ is a smooth and easily differntiable a very efficient method of solution can be obtained.
This method depends of the Taylor series expansion of the desired solution of the differentable equation. Given the initial value of the dependent variable the solution may be expanded into Taylor series expansion near the initial point.

$$y_{n+1} = y_n + \left.\frac{dy}{dx}\right|_{x=x_n} \Delta x + \frac{1}{2!}\left.\frac{d^2y}{dx^2}\right|_{x=x_n} \Delta x^2 + \mathcal{O}(\Delta x^3)$$

Basics of Numerical Analysis

If the derivatives of the dependent variable is known at the point x_n,starting from the initial values x_o, y_o iteratively the solution may be obtained at every point of the space. In fact, the first derivative is the differential equation itself,

$$\frac{dy}{dx} = f(x, y).$$

If $f(x, y)$ is a differentaible function at the point x_n, y_n, all of the higher derivatives may be obtained from the differential equation itself.

Basics of Numerical Analysis

$$(5)\quad \frac{d^2y}{dx^2} = \frac{d}{dx}\frac{dy}{dx} = \frac{d}{dx}f(x,y) = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}f$$

$$\frac{d^3y}{dx^2} = \frac{\partial^2 f}{\partial x^2} + 2f\frac{\partial^2 f}{\partial x \partial y} + f^2\frac{\partial^2 f}{\partial y^2} + \frac{\partial f}{\partial x}\frac{\partial f}{\partial y} + f(\frac{\partial f}{\partial y})^2$$

$$\vdots$$

Given the inital values x_o, y_o one can integrate the differential equation from x_o to x.

Basics of Numerical Analysis

```
double RungeKutta(double f(double x, double y), \
double x,double y,double h){
/*------------------------------------------------
     Forth order Runge-Kutta method to solve
        dy/dx = f(x,y(x))  Error is O(h^5)
------------------------------------------------
  double k1,k2,k3,k4,h2;
  h2 = 0.5 * h;
  k1 = f(x,y);  x += h2;
  k2 = f(x,y+k1*h2); k3 = f(x,y+k2*h2);
  x += h2;  k4 = f(x,y+k3*h);
  return(y+h*(k1+2*(k2+k3)+k4)/6.0L);
}/*End of function Runge-Kutta */
```