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UCRL LECTURES ON NUMERICAL ANALYSIS AND APPLIED MATHEMATICS

Lecture X

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ORDINARY DIFFERENTIAL EQUATIONS

1. Introduction

Since most of the differential equations we encounter in applications cannot be solved in closed form we must consider the other methods available. These methods include solution by infinite series, graphical solution, and direct numerical integration of the differential equation. I shall discuss the latter and give a survey of the methods available for direct numerical integration. Actually in many cases the direct integration is the best method to solve a differential equation. Although the analytic solution gives the general behaviour throughout its domain of definition the actual numerical value of the solution at required points is sometimes quite difficult to compute particularly if the solution is expressed as a transcendental equation or as an infinite series. Series solutions may be slowly convergent and the labor involved in computing the coefficients is sometimes very large. The direct numerical solution then has the advantage of giving a table of values of the particular solution desired.

I shall also discuss the applicability of computing machines to the direct solution of differential equations.

In solving a differential equation numerically there are two problems to be considered: (1) starting the solution with given initial conditions and (2) continuing the solution over an extended range of the independent variable. The methods available for continuing the solution generally require four or five successive values of the solution for equal intervals of the independent variable. Consequently, I shall first discuss methods of starting the solution. These methods in theory can solve the equation over an extended range but the computations become so cumbersome that they are only practical over a small neighborhood of the origin. The methods of starting a solution are the existence theorems of Picard and Cauchy, the method of Runge-Kutta, and the Euler method. The methods of continuing the solution are the forward integration by finite differences and Milne's method. Most equations encountered of second and higher order may be reduced to a system of first order equations by the substitutions

$$p = \frac{dy}{dx} \quad , \quad \frac{d^2y}{dx^2} = \frac{dp}{dx} = q \quad , \quad \text{etc.}$$

Likewise systems of simultaneous equations of higher order may be reduced to a system of first order equations. Consequently, the integration formulae introduced will be for a first order equation but can be applied to a system, simultaneously.

2. Picard's Method of Successive Approximations.

Consider the first order equation

$$y' = f(x, y) \tag{1}$$

with the initial condition $y(x_0) = y_0$. We may write (1) in the form

$$y(x) = y_o + \int_{x_o}^{x} f(x, y)dx \qquad (2)$$

A first approximation to the solution is

$$y_1(x) = y_o + \int_{x_o}^{x} f(x, y_o)dx$$

and, similarly, we get the following sequence of successive approximations

$$y_2(x) = y_o + \int_{x_o}^{x} f(x, y_1)dx$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$y_{n+1}(x) = y_o + \int_{x_o}^{x} f(x, y_n)dx \quad .$$

Consider now the series

$$y(x) = y_o + (y_1 - y_o) + (y_2 - y_1) + \cdots + (y_{n+1} - y_n) \quad \cdots \qquad (3)$$

for which we wish to determine conditions under which it will converge and represent the unique solution of (1). The existence theorem of Picard tells us the conditions.

<u>Theorem</u>: If $f(x, y)$ satisfies

(a) $f(x, y)$ continuous in some domain

$$R \quad , \qquad \left| f(x, y) \right| < M$$

(b) $\left| f(x, y_1) - f(x, y_2) \right| < K \left| y_1 - y_2 \right|$

then (3) is the unique solution of

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

This method is quite useful for starting the solution as the integrations do not require too much labor over a limited range. Over an extended range, however, the integrations soon become quite cumbersome.

3. Cauchy's Existence Theorem (Taylor's Series).

Consider the equation

$$y' = f(x, y) \tag{1}$$

with initial condition $y(x_o) = y_o$.

Theorem: If $f(x, y)$ is analytic in a neighborhood of (x_o, y_o) then (1) has a unique solution

$$y(x) = y_o + y'(x_o)(x - x_o) + \frac{y''(x_o)}{2!}(x - x_o)^2 + \dots .$$

The derivatives evaluated at x_o are determined by

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

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

and so on. It is obvious that this method becomes impractical unless $\left| x - x_o \right|$ is taken sufficiently small so that the higher order terms can be neglected. Consequently, this method is used only for starting the numerical solution. Generally, numerical integration formulae require at least four successive

values to start the solution and since it is desirable to keep $|x - x_o|$ small, we should compute y both to the right and left of the point x_o.

4. Method of Euler.

Another method often used for obtaining starting values is the method of Euler which merely replaces the equation $y' = f(x, y)$ by

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

so the first increment in y is

$$\Delta y_1 = f(x_o, y_o)\Delta x_1 ,$$

the second increment is then

$$\Delta y_2 = f(x_o + \Delta x_1, y_o + \Delta y_1)\Delta x_2$$

$$= f(x_1, y_1)\Delta x_2 ,$$

where

$$y_1 = y_o + \Delta y_1$$

$$y_2 = y_1 + \Delta y_2 .$$

This method is not too accurate except for very small Δx but is useful for rough work over a narrow range.

We also have the modified Euler method which is somewhat more accurate. In this method we proceed as before but improve our value several times before proceeding to the next interval. To explain further let

$$\Delta y_{11} = f(x_o, y_o)\Delta x$$

$$y_1^{(1)} = y_o + \Delta y_{11} .$$

A second approximation is then

$$\Delta y_{12} = \frac{f(x_o, y_o) + f(x_1, y_1^{(1)})}{2} \Delta x$$

and

$$y_1^{(2)} = y_o + \Delta y_{12} .$$

A third approximation would then be

$$y_1^{(3)} = y_o + \frac{f(x_o, y_o) + f(x_1, y_1^{(2)})}{2} \Delta x$$

and so on. The process is repeated until no change is produced in the value of y_1 to the number of digits retained. The first approximation of y_2 is then

$$y_2^{(1)} = y_1 + f(x_1, y_1) \Delta x$$

and the averaging process is then applied to find better approximations for y_2.

5. Runge-Kutta Method.

Consider the equation

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

with initial condition $y(x_o) = y_o$. Let $h = \Delta x$, then the increment Δy corresponding to Δx is computed from the following set of formulae.

$$k_1 = f(x_o, y_o)h , \qquad \text{(Euler method)}$$

$$k_2 = f(x_o + \frac{h}{2}, y_o + \frac{k_1}{2})h ,$$

$$k_3 = f(x_o + \frac{h}{2}, y_o + \frac{k_2}{2})h ,$$

$$k_4 = f(x_o + h, y_o + k_3)h ,$$

then

$$\Delta y_1 = \frac{1}{6} (k_1 + 2 k_2 + 2 k_3 + k_4)$$

and

$$y_1 = y_o + \Delta y_1$$

$$x_1 = x_o + h .$$

The next increment Δy_2 is computed in the same manner.

$$k_1 = f(x_1, y_1)h$$

$$k_2 = f(x_1 + \frac{h}{2} , y_1 + \frac{k_1}{2})h$$

$$k_3 = f(x_1 + \frac{h}{2} , y_1 + \frac{k_2}{2})h$$

$$k_4 = f(x_1 + h, y_1 + k_3)h$$

and

$$\Delta y_2 = \frac{1}{6} (k_1 + 2 k_2 + 2 k_3 + k_4) .$$

If $f = f(x)$ the above formulae reduce to Simpson's rule. The inherent error is also of the same order as Simpson's rule. Similar formulae for second order equations and simultaneous equations may be found in Scarborough, Numerical Mathematical Analysis. The Runge-Kutta method is excellent for starting the solution but becomes too laborious for many steps.

6. Forward Integration of First Order Equations.

The methods of forward integration are designed to continue the solution over a wide range. They are derived from interpolating polynomials which are then used to extrapolate. Consequently, several starting values

must be obtained by one of the methods already described. If the integration is required correct to a number of significant figures, then two more figures should be retained in the table.

Consider now the following table, where $q = \frac{dy}{dx} = f(x, y)$

x_o	y_o		q_o					
		Δy_o		Δq_o				
x_1	y_1		q_1		$\Delta^2 q_o$			
		Δy_1		Δq_1		$\Delta^3 q_o$		
x_2	y_2		q_2		$\Delta^2 q_1$		$\Delta^4 q_o$	
		Δy_2		Δq_2		$\Delta^3 q_1$		$\Delta^5 q_o$
x_3	y_3		q_3		$\Delta^2 q_2$		$\Delta^4 q_1$	
		Δy_3		Δq_3		$\Delta^3 q_2$		$\Delta^5 q_1$
x_4	y_4		q_4		$\Delta^2 q_3$		$\Delta^4 q_2$	
		Δy_4		Δq_4		$\Delta^3 q_3$		
x_5	y_5		q_5		$\Delta^2 q_4$			
		Δy_5		Δq_5				
x_6	y_6		q_6					

The $x_o, x_1, x_2, \ldots$ are defined by the chosen increment of the independent variable. The increment, $\Delta x = h$, is a constant. It is better to keep the increment in x small and thus simplify the formulae of integration. If the increment is too large the higher order differences in q become larger

and more terms are needed for convergence. If this does happen it is best to decrease the increment in x. When the increment $(\Delta x = h)$ is halved during an integration the intermediate values of q may be computed using Bessel's interpolation formula

$$q_{n,n+1} = \tfrac{1}{2}(q_n + q_{n+1}) - \frac{1}{16}(\Delta^2 q_n + \Delta^2 q_{n+1}) + \frac{3}{256}(\Delta^4 q_{n-1} + \Delta^4 q_{n-2}) .$$

The intermediate values of y may be computed from the same formula or from the integration formula or both.

In the table (1) the $y_0, \ldots, y_5$ are given by the starting values obtained by one of the previous methods. The $q_0, \ldots, q_5$ are calculated from the differential equation in sequence form

$$q_i = f(x_i, y_i) .$$

To continue the solution we next want y_6 so we must find Δy_5 since

$$y_6 = y_5 + \Delta y_5 .$$

The increment Δy_5 is then obtained from the forward integration formula,

$$\Delta y_n = h(q_{n-1} + \frac{1}{2}\Delta q_{n-2} + \frac{5}{12}\Delta^2 q_{n-3} + \frac{3}{8}\Delta^3 q_{n-4} + \frac{251}{720}\Delta^4 q_{n-5} + \ldots) .$$

We then calculate $q_6 = f(x_6, y_6)$ and proceed to difference q, i.e., obtain

$$\Delta q_5 , \ \Delta^2 q_4, \ \Delta^3 q_3, \ \Delta^4 q_2 .$$

Before proceeding to calculate Δy_6 we should check our value for Δy_5 by the checking formula

$$\Delta y_n = h(q_{n+1} - \frac{1}{2}\Delta q_n - \frac{1}{12}\Delta^2 q_{n-1} - \frac{1}{24}\Delta^3 q_{n-2} - \frac{19}{720}\Delta^4 q_{n-3} \ldots)$$

which makes use of our new values.

The first error term is $\frac{h}{3}\Delta^5 q_{n-6}$ which should be kept small enough so as not to affect the accuracy required.

This method of integrating forward using differences is called the Adams-Bashforth method. There are of course several other integration formulae using differences which are described in the references, but this is the only one which we shall study in detail.

7. Milne's Method.

Another method for continuing the solution over an extended range is due to Milne. It does not require a difference table, but uses two quadrature formulas, one for integrating ahead by extrapolation and the other for checking the new value. The formulae are derived from Newton's interpolation formula. Milne's method requires at least four starting values.

Let y_0, y_1, y_2, y_3 be the four starting values. The derivatives q_0, q_1, q_2, q_3 can be calculated from $q_i = \left(\frac{dy}{dx}\right)_i = f(x_i, y_i)$. Denote the increment in x by h. The next value, y_4, is calculated by using the integration formula

$$y_n^{(1)} = y_{n-4} + \frac{4}{3} h \left[2\, q_{n-1} - q_{n-2} + 2\, q_{n-3} \right] \quad . \qquad (1)$$

The error in this value is at most $\frac{1}{3} h \Delta^4 q_{n-1}$. The new value $y_4^{(1)}$ is now checked with the formula

$$y_n^{(2)} = y_{n-2} + \frac{1}{3} h \left[q_{n-2} + 4\, q_{n-1} + q_n^{(1)} \right] \qquad (2)$$

where

$$q_n^{(1)} = f(x_n, y_n^{(1)})$$

The error in this corrected value is at most $\frac{1}{90} h \Delta^4 q_{n-1}$. This process should be repeated until two values of y agree to the desired number of figures. The integration should then be continued. Formula (2) is actually Simpson's rule for integration. Milne's method is fast and reasonably accurate. If, however, substitution of x and y into the differential equation to obtain q is a complicated computation then the repeated corrections to y and subsequent calculation of q can become tedious. Generally speaking though it is much faster than the difference methods.

8. Equations of Second and Higher Order and Simultaneous Equations.

The methods which have been discussed for first order equations can all be applied to equations of higher order and simultaneous equations. A differential equation of higher order can be reduced to a system of first order equations by introducing new variables. Consider

$$\frac{d^n y}{dx^n} = f(x, y, y', y'', \ldots, y^{(n-1)}) \qquad (1)$$

with initial conditions

$$y(x_o) = y_o \;, \quad y'(x_o) = y'_o \;, \quad \ldots \;, \quad y^{(n-1)}(x_o) = y_o^{(n-1)}$$

The equation (1) may be reduced to the system

$$\begin{aligned} y_1 &= \frac{dy}{dx} \\ y_2 &= \frac{dy_1}{dx} \\ y_3 &= \frac{dy_2}{dx} \\ &\vdots \\ y_{n-1} &= \frac{dy_{n-2}}{dx} \quad ; \quad \frac{dy_{n-1}}{dx} = f(x, y, y_1, y_2, \ldots, y_{n-1}) \,. \end{aligned} \qquad (2)$$

Let us consider a difference table for the equation

$$\frac{d^2y}{dx^2} = f(x, y, y') \tag{3}$$

with initial conditions $y(x_o) = y_o$, $y'(x_o) = y'_o$. The system we shall solve is

$$\frac{dy}{dx} = p \tag{4}$$

$$q = \frac{dp}{dx} = f(x, y, p)$$

with initial conditions $y(x_o) = y_o$, $p(x_o) = y'_o = p_o$. The difference table in accordance with the method of Section 6 is then

x_o	y_o		p_o				q_o			
		Δy_o		Δp_o				Δq_o		
x_1	y_1		p_1		$\Delta^2 p_o$		q_1		$\Delta^2 q_o$	
		Δy_1		Δp_1		$\Delta^3 p_o$		Δq_1		$\Delta^3 q_o$
x_2	y_2		p_2		$\Delta^2 p_1$		$\Delta^4 p_o$	q_2		$\Delta^2 q_1$		$\Delta^4 q_o$
		Δy_2		Δp_2		$\Delta^3 p_1$		Δq_2		$\Delta^3 q_1$
x_3	y_3		p_3		$\Delta^2 p_2$		$\Delta^4 p_1$	q_3		$\Delta^2 q_2$		$\Delta^4 q_1$
		Δy_3		Δp_3		$\Delta^3 p_2$		Δq_3		$\Delta^3 q_2$
x_4	y_4		p_4		$\Delta^2 p_3$			q_4		$\Delta^2 q_3$	
		Δy_4		Δp_4				Δq_4		
x_5	y_5		p_5					q_5			

So for integrating ahead we have with $\Delta x = h$

$$\Delta p_n = h(q_{n-1} + \frac{1}{2}\Delta q_{n-2} + \frac{5}{12}\Delta^2 q_{n-3} + \frac{3}{8}\Delta^3 q_{n-4} + \frac{251}{720}\Delta^4 q_{n-5} + \dots)$$

$$\Delta y_n = h(p_{n-1} + \frac{1}{2}\Delta p_{n-2} + \frac{5}{12}\Delta^2 p_{n-3} + \frac{3}{8}\Delta^3 p_{n-4} + \frac{251}{720}\Delta^4 p_{n-5} + \dots)$$

and for checking

$$\Delta p_n = h(q_{n+1} - \frac{1}{2}\Delta q_n - \frac{1}{12}\Delta^2 q_{n-1} - \frac{1}{24}\Delta^3 q_{n-2} - \frac{19}{720}\Delta^4 q_{n-3} - \dots)$$

$$\Delta y_n = h(p_{n+1} - \frac{1}{2}\Delta p_n - \frac{1}{12}\Delta^2 p_{n-1} - \frac{1}{24}\Delta^3 p_{n-2} - \frac{19}{720}\Delta^4 p_{n-3} - \dots) .$$

Milne's method and all the starting techniques can be applied to system (4) also in the obvious way. Simultaneous equations are solved in this manner also.

9. A Method for Integrating Equations of the Type $d^2y/dx^2 = f(x, y)$ Where the Value of dy/dx Is Not Required.

A special method which applies to equations where the first derivative does not appear explicitly is available. This method is particularly useful for calculating equations of motion of a charged particle moving under the force of an electric field. The equation

$$M\ddot{x} = e\,E_x(x, t)$$

is of the form we are discussing. Also equations of the form

$$\frac{d^2y}{dx^2} + p(x)\frac{dy}{dx} + q(x)y = r(x)$$

can be transformed by

$$z = y \exp\left(\tfrac{1}{2} \int_{x_0}^{x} p(x)dx\right)$$

to the equation

$$\frac{d^2 z}{dx^2} = b(x)z + c(x)$$

and this equation can be solved by the method to be described. The advantages of this method are that it is fast and requires only three starting values.

Consider the difference table for $q = y'' = f(x, y)$ with initial conditions $y(x_0) = y_0$, $y'(x_0) = y'_0$.

x_0	y_0			q_0		
		Δy_0			Δq_0	
x_1	y_1		$\Delta^2 y_0$	q_1		$\Delta^2 q_0$
		Δy_1			Δq_1	
x_2	y_2		$\Delta^2 y_1$	q_2		$\Delta^2 q_1$
		Δy_2			Δq_2	
x_3	y_3		$\Delta^2 y_2$	q_3		$\Delta^2 q_2$
		Δy_3			Δq_3	
x_4	y_4			q_4		

We may integrate ahead with the equation (1), with $\Delta x = h$

$$y_{n+1} - 2y_n + y_{n-1} = \Delta^2 y_{n-1} = h^2 \left[q_n + \frac{1}{12} \Delta^2 q_{n-2}\right] \qquad (1)$$

and check the value we obtain with

$$y_{n+1} - 2\,y_n + y_{n-1} = \Delta^2 y_{n-1} = h^2\left[q_n + \frac{1}{12}\Delta^2 q_{n-1}\right] \qquad (2)$$

The first error term in equation (1) is $-\frac{1}{12}\Delta^5 q_n$ whereas for equation (2) it is $\frac{1}{240}\Delta^6 q_n$. The integration can be speeded up then if equation (2) is used for integrating ahead as well as checking. This means a value for $\Delta^2 q_{n-1}$ must be estimated but this can usually be done with practice and it is a better approximation than $\Delta^2 q_{n-2}$ which is the value suggested by equation (1).

10. Application of Computing Machines to the Solution of Ordinary Differential Equations.

All of the methods discussed are greatly facilitated by the use of a desk calculator to perform the required arithmetic operations. These methods are also the ones used in solving differential equations with a high-speed digital computer. These modern high-speed machines perform only the ordinary arithmetic operations. Consequently, the problem must be put in numerical analysis form. The advantage of these machines is that the operations are performed with great speeds automatically. That is the numbers can be stored in a memory unit along with coded commands which tell the arithmetic unit what operations to perform on the numbers. The solutions of large systems of equations for many sets of initial conditions over a wide range are made possible with the use of these machines.

11. The Differential Analyzer.

The differential analyzer is an instrument for evaluating the solutions of systems of ordinary differential equations. It consists of a number of integrators which can be connected together so as to solve an ordinary

differential equation directly for given boundary conditions. It comes under the class of analog computers in that the differential equation to be solved is used to describe a mechanical or electrical system which is then constructed on the differential analyzer. The U.C.R.L. differential analyzer is a mechanical machine. That is, the functions are represented by rotations and the integrators are continuously variable gears. The connection system is an electro-mechanical one using synchro motors. For a more complete description of this machine see references (3) and (4).

12. References.

All of the methods described in this report with special cases and numerical examples are found in the following:

12.1 Levy, H. and Baggott, E. A., Numerical Solutions of Differential Equations, 1st. Am. Ed., 1950, Dover Publications, Inc.

12.2 Scarborough, J. B., Numerical Mathematical Analysis, 2nd Ed., 1950, The Johns Hopkins Press.

12.3 Sorenson, E., "Construction and Maintenance Report on the UCRL Differential Analyzer", UCRL-1717.

12.4 Killeen, J., "Application and Operation of the UCRL Differential Analyzer", UCRL report in progress.