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TITLE: RUNGE-KUTTA INTEGRATION

PURPOSE: To give a brief description of the Runge-Kutta process for point-wise integration of systems of differential equations.

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CONTENTS:

This survey has 9 parts:

I Purpose of Method

To solve a simultaneous set of n first order differential equations $y_i' = f(x, y_1, y_2, \cdots y_n)$, given only one initial value for each y_i at x_o.

II Geometric Principle

Consider the equation $y' = f(x, y)$, where (x_o, y_o) is known. Given h, find k such that $(x_o + h, y_o + k)$ is on the curve. The first approximation to k is given by drawing a line from (x_o, y_o) with slope $\left.\frac{dy}{dx}\right|_{x=x_o}$ and finding $(x_o + h, y_o + k_1)$ on this line. k_2 is found by picking an intermediate point x_1, finding y_1 on the line, then creating a new line through (x_o, y_o) with slope $\left.\frac{dy}{dx}\right|_{x=x_1}$, then finding $(x_o + h, y_o + k_2)$ on the new line. This process is repeated successively until a predetermined number of k_i have been found. Then k is taken as a weighted average of these k_i.

III Derivation for One Equation

Given $y_o' = f(x_o, y_o)$, find y such that $y' = f(x, y)$.

$$y'' = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx} = f_x + f_y f$$

$$y''' = \frac{\partial y''}{\partial x} + \frac{\partial y''}{\partial y}\frac{dy}{dx} = f_{xx} + 2f_{xy}f + f_{yy}f^2 + (f_x + f_y f)\, f_y$$

The Taylor Series about x_o is:

$$y = y_o + (x - x_o)\, y_o' + \frac{1}{2!}(x - x_o)^2 y_o'' + \frac{1}{3!}(x - x_o)^3 y_o''' + \cdots$$

Let $h = x - x_o$, $\Delta y = y - y_o$,

$$(*) \qquad \Delta y = f_o h + \frac{1}{2} h^2 (f_x + f_y f)\Big|_{(x_o, y_o)} + \frac{1}{6} h^3 \Big[f_{xx} + 2f_{xy}f + f_{yy}f^2 + (f_x + f_y f)\, f_y \Big]\Big|_{(x_o, y_o)} + \cdots$$

Let $k_1 = hf(x_o, y_o)$

$k_2 = hf(x_o + mh, y_o + mk_1)$

$k_3 = hf(x_o + \lambda h, y_o + \rho k_2 + (\lambda - \rho) k_1)$

Where m, λ, ρ are constants.

Taylor's Formula is:

$$f(x_o + p, y_o + q) = f(x_o, y_o) + f_x(x_o, y_o)\, p + f_y(x_o, y_o)\, q + \frac{1}{2}\left[f_{xx}(x_o, y_o)\, p^2 + 2 f_{xy}(x_o, y_o)\, pq + f_{yy}(x_o, y_o)\, q^2\right] + \cdots$$

Expanding k_2, k_3 by Taylor's Formula,

$$k_1 = h\, f(x_o, y_o)$$

$$k_2 = h\left\{f(x_o, y_o) + mh\, f_x(x_o, y_o) + mk_1\, f_y(x_o, y_o) + \frac{1}{2}\left[(mh)^2 f_{xx}(x_o, y_o) + 2m^2h\, k_1\, f_{xy}(x_o, y_o) + (mk_1)^2 f_{yy}(x_o, y_o)\right] + \cdots\right\}$$

$$k_3 = h\left\{f(x_o, y_o) + \lambda h\, f(x_o, y_o) + \left[\rho k_2 + (\lambda - \rho) k_1\right] f_y(x_o, y_o) + \frac{1}{2}\left\{(\lambda h)^2 f_{xx}(x_o, y_o) + 2\lambda h\left[\rho k_2 + (\lambda - \rho) k_1\right] f_{xy}(x_o, y_o) + \left[\rho k_2 + (\lambda - \rho) k_1\right]^2 f_{yy}(x_o, y_o)\right\} + \cdots\right\}$$

By substituting for k_1, k_2 and truncating to h^3, get:

$$k_1 = h\, f(x_o, y_o)$$

$$k_2 = h\, f(x_o, y_o) + h^2 m (f_x + f_y f)\Big|_{(x_o, y_o)} + \frac{1}{2} m^2 h^3 (f_{xx} + 2 f_{xy} f + f_{yy} f^2)\Big|_{(x_o, y_o)}$$

$$k_3 = hf(x_o, y_o) + \lambda h^2 (f_x + f_y f)\Big|_{(x_o, y_o)} + \frac{1}{2} h^3 \left[\lambda^2 (f_{xx} + 2f_{xy} f + f_{yy} f^2) + 2m\rho (f_x + f_y f) f_y\right]\Big|_{(x_o, y_o)}$$

Form the weighted mean:

(**) $$\bar{K} = ak_1 + bk_2 + ck_3$$

where a, b, c are arbitrary constants.

Forming this sum and setting $\bar{K} = \Delta y$, ie, equating coefficients in (*) and (**), one gets:

$$a + b + c = 1$$

$$bm + c\lambda = \tfrac{1}{2}$$

$$bm^2 + c\lambda^2 = 1/3$$

$$c\rho m = 1/6$$

We now have four equations in six unknowns.

Upon solving this system for a, b, c, m, λ, ρ, get $\Delta y = ak_1 + bk_2 + ck_3$. This agrees with the Taylor expansion of Δy as far as the h^3 term. The error is on the order of h^4.

IV Ease of Computation

Four equations in six unknowns gives 2 degrees of freedom. By assigning 2 values appropriately, one can get particularly simple formulas. A widely used set of four k's is:

$$k_1 = h\ f\ (x_o, y_o)$$

$$k_2 = h\ f\ (x + \tfrac{1}{2} h,\ y + \tfrac{1}{2} k_1)$$

$$k_3 = h\ f\ (x + \tfrac{1}{2} h,\ y + \tfrac{1}{2} k_2)$$

$$k_4 = h\ f\ (x + h,\ y + k_3)$$

$$\Delta y = 1/6\ (k_1 + 2k_2 + 2k_3 + k_4)$$

For other simple formulas, see [4], P. 186.

V Generalization to More Equations

Consider the generalization to n simultaneous differential equations:

$$\frac{dy_i}{dx} = f_i\ (x, y_1, y_2, \cdots, y_n)\ (i = 1, \cdots, n)$$

Using the simple formula described above, we get:

1. $k_{i1} = hf_i\ (x_o, y_{1_o}, y_{2_o}, \cdots, y_{n_o})$

2. $k_{i2} = hf_i\ (x_o + \frac{1}{2} h, y_{1_o} + \frac{1}{2} k_{11}, y_{2_o} + \frac{1}{2} k_{21}, \cdots)$

3. $k_{i3} = hf_i\ (x_o + \frac{1}{2} h, y_{1_o} + \frac{1}{2} k_{12}, y_{2_o} + \frac{1}{2} k_{22}, \cdots)$

4. $k_{i4} = hf_i\ (x_o + h, y_{1_o} + k_{13}, y_{2_o} + k_{23}, \cdots)$

then $\Delta y_i = 1/6\ (k_{i1} + 2\ k_{i2} + 2\ k_{i3} + k_{i4})\quad (i = 1, \cdots n)$

VI Modification by S. Gill

In [2], S. Gill uses the 2 degrees of freedom to minimize the amount of storage required for intermediate computations. If there are n equations, Gill succeeds in reducing the order of the number of storage registers from 4n to 3n (from 8n to 6n for floating point computations).

VII Accuracy

To get higher orders of accuracy, one needs to use a larger number of k's in forming the average $\overline{K}$. Four k's will give fourth-order accuracy, but fifth-order accuracy requires six k's. Every additional k greatly increases the number of computations since an additional term in Taylor's Formula is required, plus an additional substitution into each f_i.

VIII Recommendation

This method is particularly useful in obtaining starting values, since only one initial condition is required; more sensitive methods can then be used to get successive points to greater accuracy. Furthermore, the large number of computations makes this method unwieldy for many points.

The modification by S. Gill is widely used and is recommended.

IX Bibliography

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2. Gill, S., A Process for the Step-by-Step Integration Of Differential Equations in an Automatic Digital Computing Machine, 3 June 1950.

3. Kopal, Zdenek, Numerical Analysis, PP. 195-214, 1955

4. Kunz, Kaiser S., Numerical Analysis, PP. 183-189, 1957

REFERENCES: See Bibliography

INFORMATION TO: All Concerned

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