Numerical Integration of Differential Equations

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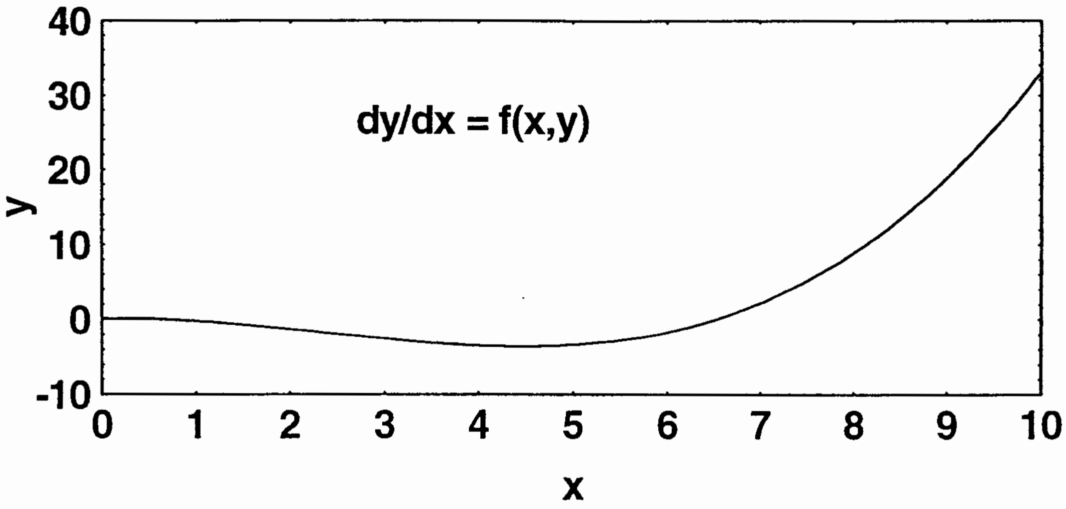
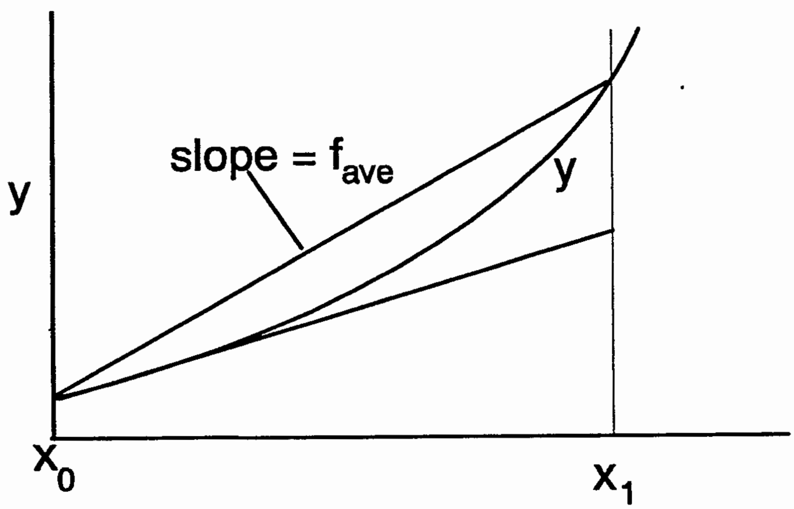


Consider the differential equation: $\frac{dy}{dx} = f(x,y)$ subject to y(a) = b

The condition $y(a) = b$ is called an *initial condition.* a and b are known numbers.

The approach to integrate the differential equation numerically is to start at $x = a$ where we know the solution, $y = b$. Then we move to $x = a + \Delta x$. The solution at that point is: $y = a + f_{ave}\Delta x$, where f_{ave} is the average value of $\frac{dy}{dx}$ over the interval from a to $a + \Delta x$. Then we proceed in the same way to obtain $y(a + 2\Delta x)$. The accuracy of the numerical solution depends of the accuracy of the estimate of f_{ave}. The various ways of making this estimate are called *rules* or *methods.* We will index the points at which y is determined by i so the computed values are $y_0, y_1, y_2, ...$ at values of x: $x_0, x_1, x_2, ...$ The simplest method is Euler's Method.



Euler's Method In Euler's method, to estimate y_{i+1}, f_{ave} is approximated by its value at (x_i, y_i) or its value at (x_{i+1}, y_i) The former case is called the forward Euler Method and the latter case is called the backward Euler Method.

For the forward Euler Method: $y_{i+1} \approx y_i + f(x_i, y_i)(x_{i+1} - x_i)$

Expanding y in a Taylor series about x_o gives:

$$y(x) = y(x_0) + (x - x_0)y'(x_0) + \frac{(x - x_0)^2}{2} y''(x_0) + \dots$$

The error,ϵ, for one step in the solution by the Euler Method can be obtained from the first omitted term in the above Taylor series:

$$\epsilon = \frac{(x - x_0)^2}{2} \frac{d^2y}{dx^2}$$

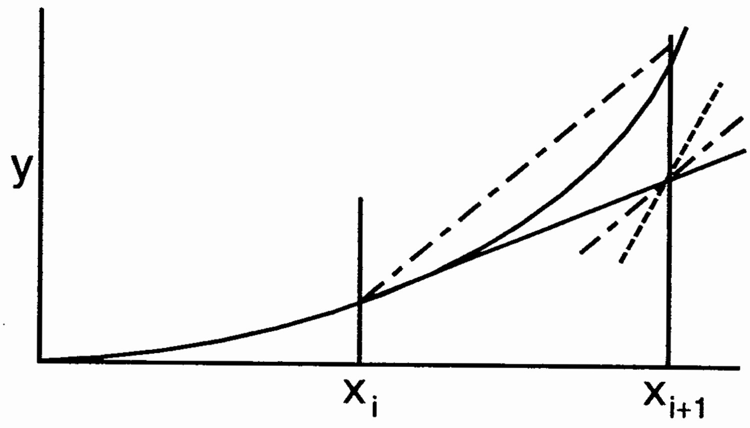
The meaning of the error depends on the value of x for which $\frac{d^2y}{dx^2}$ is evaluated. There is one point in the interval for which the computed error is exact. However, the location of that point is not known. If we take the absolute value of the maximum value of $\frac{d^2y}{dx^2}$ in the interval, the result is an upper bound on the error. ϵ is called the local error for the interval. The total error for the entire interval is called the global error. The sum of the values of ϵ for all the intervals is an upper bound on the global error. For demonstration purposes, if we have a differential equation that can be solved analytically, the exact global error can be calculated. It can be shown that the global error diminishes as the step (interval) size, Δx, is made smaller.

Modified Euler's Method

The forward Euler method uses the derivative at the initial point of the interval. The backward Euler method uses the derivative close to the end point of the interval. A numerical solution with improved accuracy is obtained by using the average of the derivative at the initially computed end points.

$$y_{i+1} \approx y_i + \frac{x_{i+1} - x_i}{2} \{y'(x_i, y_i) + y'[x_{i+1}, y_i + (x_{i+1} - x_i)\, y'(x_i, y_i)]\}$$

Modified Euler's Method (continued)



For each successive interval, the steps are:

1. Evaluate the slope $[y'(x_i, y_i)]$ at the start of the interval.
2. Estimate y_{i+1} at the end of the interval using Euler's Method.
3. Evaluate the slope, $y'[x_{i+1}, y_i + (x_{i+1} - x_i)y'(x_i, y_i)]$, at the end of the interval.
4. Calculate the average of the two slopes,y'_{ave} from steps 1 and 3.
5. Calculate a revised value of y_{i+1} using the average slope, $y_{i+1} = y_i + (x_{i+1} - x_i)y'_{ave}$.

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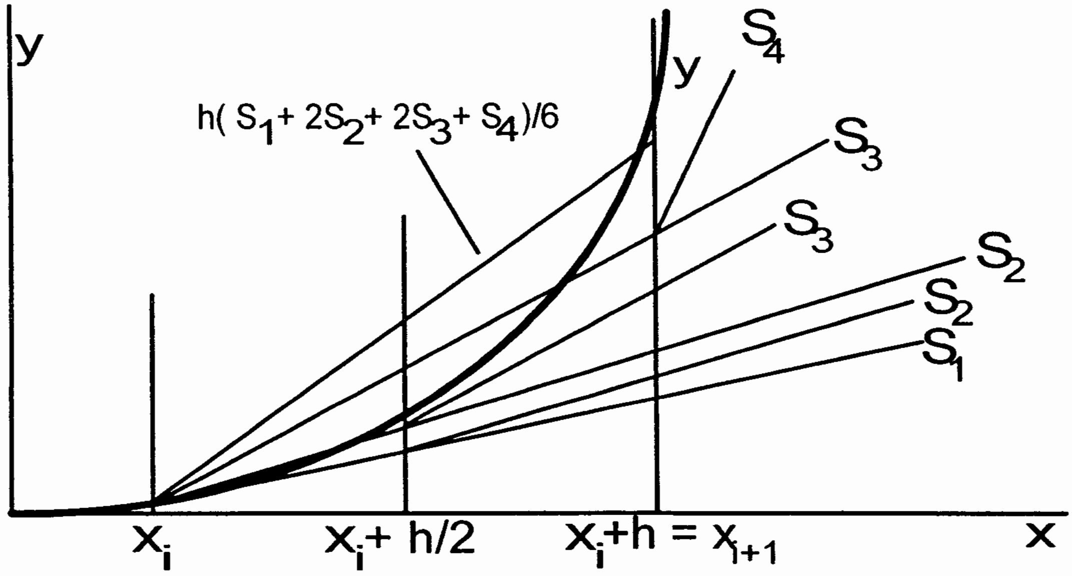
Fourth Order Runge Kutta Method



The fourth order Runge Kutta method estimates the average value of $f = \frac{dy}{dx}$ in an interval of length h in terms of values of f at four locations in (x, y) space. If the initial point of the interval is (x_i, y_i), one derivative is evaluated there, one is at $x = x_i + h$ and two are at $x = x_i + h/2$, for two different values of y. If $\frac{dy}{dx}$ depends only on x and not on y, the two intermediate values of f are the same.

The four slopes are:

$$s_1 = f(x_i, y_i)$$

$$s_2 = f(x_i + 0.5h, y_i + 0.5hs_1)$$

$$s_3 = f(x_i + 0.5h, y_i + 0.5hs_2)$$

$$s_4 = f(x_i + h, y_i + hs_3)$$

Then the value of y at the end of the interval is estimated as:

$$y_{i+1} = y_i + \frac{h}{6}(s_1 + 2s_2 + 2s_3 + s_4)$$

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Predictor-Corrector Methods

Two difficulties with high order Runge Kutta methods are the computation time required to compute several values of the derivative at each time step and the exact error is unknown. Predictor-corrector methods allow fewer computations if the number of corrector steps is limited and allow iterations of the corrector step converging to a very accurate solution if the required computation time is available.

The approach with a predictor-corrector method involves two steps. The first is a prediction step using any integration method and the second is the correction step which improves upon the prediction. The process is explained here using the simplest rules: the Forward Euler Method for the prediction step and the trapezoidal rule for the correction step. The equation to be solved is: $\frac{dy}{dx} = f(x,y)$. Consider the interval from index i to index $i+1$ with $x_{i+1} - x_i = h$. The prediction step is:

$$y_{i+1,0} = y_{i,*} + hf_{i,*}$$

The second subscript on the left hand side, 0 indicates that there have been zero correction steps (or trials). The second subscripts, $*$, on the right hand side means that the subscripted quantities are for the final step; in this case for the i^{th} integration step.

Now we use the trapezoidal rule to correct the estimate of y_{i+1}.

$$y_{i+1,1} = y_{i,*} + \frac{h}{2}\left[f_{i,*} + f_{i+1,0}\right]$$

The rightmost term can be evaluated since we know $y_{i+1,0}$ from the previous prediction step. We can refine the estimate, using the value of y_{i+1} from the prior correction step.

$$y_{i+1,j} = y_{i,*} + \frac{h}{2}\left[f_{i,*} + f_{i+1,j-1}\right]$$

This process can be continued until y converges. The converged result is the exact solution to the numerical problem as posed, but is not necessarily the solution to the actual continuous mathematics solution. In this case, the numerical problem is based on the average derivative over the interval being the average of its value at the two ends. This is not exactly correct for differential equations in general.

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Higher Order Differential Equations

$$\text{Consider the equation:}\quad \frac{d^2y}{dx^2} + f_1(x,y)\frac{dy}{dx} + f_o(x,y)\,y = g(x,y)$$

$$\text{Let:}\quad \frac{dy}{dx} = z$$

$$\text{Then:}\quad \frac{dz}{dx} = -f_1(x,y)\,z - f_o(x,y)\,y + g(x,y)$$

When we use an integration rule, at each step it is applied to the two equations above and everything else proceeds as it does for a first order differential equation.

The same approach can be used for equations of higher order. For example:

$$\frac{d^3y}{dx^3} + f_2(x,y)\frac{d^2y}{dx^2} + f_1(x,y)\frac{dy}{dx} + f_o(x,y)\,y = g(x,y)$$

Make the following definitions:

$$\frac{dy}{dx} = z$$

$$\frac{dz}{dx} = \frac{d^2y}{dx^2} = w$$

$$\text{Then:}\quad \frac{dw}{dx} = -f_2(x,y)\,w - f_1(x,y)\,z - f_0(x,y)\,y + g(x,y)$$

In this case, the integration rule is applied to three equations at each step.

Review and Extension

Simple Example

$$\text{Suppose: } \frac{d^2y}{dt^2} + f(y,t)\frac{dy}{dt} + g(y,t)\,y = h(y,t)$$

$$\frac{d^2y}{dt^2} = -f(y,t)\frac{dy}{dt} - g(y,t)\,y + h(y,t)$$

$$\text{Let: } q(y,t) = \frac{dy}{dt}$$

$$\frac{dq}{dt} = -f(y,t)\,q - g(y,t)\,y + h(y,t)$$

Consider the simplest integration rule: Forward Euler Integration

$$q(t+\delta t) = q(t) + [-f(y(t),t)\,q(t) - g(y(t),t)\,y(t) + h(y(t),t)]\,\delta t$$

$$y(t+\delta t) = y(t) + q(t)\,\delta t$$

Slightly More Complicated Example

$$\frac{\partial^2 y(x,t)}{\partial t^2} + f(x,y,t)\frac{\partial y(x,t)}{\partial t} + g(x,y,t)y(x,t)m = h(x,y,t)$$

Follow the above procedure for each (fixed) value of x.

$$\frac{\partial^2 y(x,t)}{\partial t^2} = -f(x,y,t)\frac{\partial y(x,t)}{\partial t} - g(x,y,t)\,y + h(x,y,t)$$

$$\text{Let: } q(x,y,t) = \frac{\partial y(x,t)}{\partial t}$$

$$\frac{\partial q(x,y,t)}{\partial t} = -f(x,y(x,t),t)\,q(x,y,t) - g(x,y,t)\,y(x,y,t) + h(x,y,t)$$

Now we do the numerical integration by the Euler Method. Any other method can also be used.

$$q(x,y,t+\delta t) = q(x,y,t) + [-f(x,y(x,t),t)\,q(x,y(x,t),t) - g(x,y(x,t),t)\,y(x,t) + h(x,y(x,t),t)]\,\delta t$$

$$y(x,t+\delta t) = y(x,t) + q(x,y,t)\,\delta t$$