Taylor Series for Differential Equation Solvers' Local Error

The *Taylor Series* of an infinitely differentiable vector-valued function y(t) of a scalar t is

$$y(t) = y(0) + t\cdot y'(0) + t^2\cdot y''(0)/2 + t^3\cdot y'''(0)/6 + t^4\cdot y''''(0)/24 + \dots .$$

These derivatives can be computed for a solution of the *Initial Value Problem*

" $y(0) = y_0$ is given, and $y'(t) = f(y(t))$ for all $t \ge 0$ "

from the derivatives of the given vector-valued function $f(y)$. In fact, from the *Chain Rule,*

$$y' = f,\ y'' = f'\cdot f,\ y''' = f''\cdot f\cdot f + f'^2\cdot f,\ \ y'''' = f'''\cdot f\cdot f\cdot f + 3f''\cdot f'\cdot f\cdot f + f'\cdot f''\cdot f\cdot f + f'^3\cdot f,\ \dots .$$

Then each derivative of y(t) can be evaluated at t = 0 by evaluating each derivative of $f(y)$ at $y = y(0) = y_0$. Note that the higher derivatives of f are *symmetric multilinear operators*; for instance, $f''(y)$ is a *symmetric bilinear* operator: $f''\cdot u\cdot v = f''\cdot v\cdot u$ is a vector-valued linear function of each vector u and v separately. Because linear operators do not necessarily commute, $f''\cdot f'\cdot f\cdot f \ne f'\cdot f''\cdot f\cdot f$ in general, though they are equal if y's vector space is one-dimensional. If y's vector space is N-dimensional, then y and f can be represented by column vectors each with N components; f' by a matrix with N^2 components; f'' by an array with N^3 components of which at most $(N+1)N^2/2$ can be distinct; f''' by an array of N^4 components … . Higher derivatives' arrays become huge when N is large.

Normally the Taylor series would be used to obtain y(t+h) from y(t) for any sufficiently small stepsize h :

$$y(t+h) = y(t) + h\cdot y'(t) + h^2\cdot y''(t)/2 + h^3\cdot y'''(t)/6 + h^4\cdot y''''(t)/24 + \dots ,$$

in which the derivatives dy(t+h)/dh etc. are computed at h = 0 from the same formulas

$$y' = f,\ \ y'' = f'\cdot f,\ \ y''' = f''\cdot f\cdot f + f'^2\cdot f,\ \ y'''' = f'''\cdot f\cdot f\cdot f + 3f''\cdot f'\cdot f\cdot f + f'\cdot f''\cdot f\cdot f + f'^3\cdot f,\ \dots$$

as before except that now $f(y)$ and its derivatives are computed at y = y(t) .

A similar process generates a formal series for any one-step numerical method's formula that advances an approximate solution y = y(t) through one step h to Y = Y(t+h) , but now we differentiate with respect to h instead of t to get

$$Y(t+h) = y + h\cdot Y' + h^2\cdot Y''/2 + h^3\cdot Y'''/6 + h^4\cdot Y''''/24 + \dots$$

in which y = y(t) and the derivatives Y' etc. are derivatives of Y(t+h) with respect to h evaluated at h = 0 . These derivatives depend upon the numerical method's formula. For example, take the (implicit) *Trapezoidal Rule* $Y = y + h\cdot(f(y) + f(Y))/2$. Now, at t+h ,

$$Y' = (f(y) + f(Y))/2 + h\cdot f'(Y)\cdot Y'/2 ,$$
$$Y'' = f'(Y)\cdot Y' + h\cdot(\ f''(Y)\cdot Y'\cdot Y' + f'(Y)\cdot Y''\ )/2 ,$$
$$Y''' = 3f''(Y)\cdot Y'\cdot Y'/2 + f'(Y)\cdot Y''/2 + h\cdot(\ f'''(Y)\cdot Y'\cdot Y'\cdot Y' + \dots\ )/2 , \quad \text{etc.}$$

Here every instance of Y or its derivatives is evaluated at t+h . For the Taylor series we set h = 0 in the foregoing formulas and substitute for derivatives of Y in succession to get

$$Y' = f,\ \ Y'' = f'\cdot f,\ \ Y''' = (\ 3f''\cdot f + f'^2\ )\cdot f/2,\ \ \dots$$

in which now the derivatives of Y are evaluated at t , and f and its derivatives are evaluated at y(t) . Hence, the computed approximation

$$Y(t+h) = y(t) + h\cdot f + h^2\cdot f'\cdot f/2 + h^3\cdot(\ 3f''\cdot f + f'^2\ )\cdot f/12\ + \dots$$

can be compared with the local solution

$$y(t+h) = y(t) + h\cdot f + h^2\cdot f'\cdot f/2 + h^3\cdot(\ f''\cdot f + f'^2\ )\cdot f/6 + \dots$$

to reveal the 2nd-order Trapezoidal Rule's local truncation error

$$y(t+h) - Y(t+h) = h^3\cdot(\ f'^2 - f''\cdot f)\cdot f/12 + \dots .$$

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Another example is the (implicit) *Midpoint Rule* $Y = y + h \cdot f((y+Y)/2)$. At t+h ,

$$Y' = f((y+Y)/2) + h \cdot f'((y+Y)/2) \cdot Y'/2 ,$$
$$Y'' = f'((y+Y)/2) \cdot Y' + h \cdot (f''((y+Y)/2) \cdot Y' \cdot Y'/4 + f'((y+Y)/2) \cdot Y''/2) ,$$
$$Y''' = 3f''((y+Y)/2) \cdot Y' \cdot Y'/4 + 3f'((y+Y)/2) \cdot Y''/2 + h \cdot (f''' \dots) , \text{ etc.}$$

Setting $h = 0$ and substituting for derivatives of Y in succession yields

$$Y' = f , \quad Y'' = f' \cdot f , \quad Y''' = (3f'' \cdot f + 6f'^2) \cdot f/4 , \quad \dots$$

in which now the derivatives of Y are evaluated at t , and f and its derivatives are evaluated at y(t) . Hence, by comparison with the Taylor series for y(t+h) we find the 2nd-order Midpoint Rule's local truncation error to be

$$y(t+h) - Y(t+h) = h^3 \cdot (f'' \cdot f - 2f'^2) \cdot f/24 + \dots .$$

The foregoing manipulations are tedious enough that only a computerized algebra system should perform them. However, programming *Maple* or *Mathematica* or *Derive* to perform them has been more difficult than it should be. At least some of the difficulty arises, I think, because these languages disallow declaration of a variable's linguistic *Type*. Besides the derivatives' non-commutative partially associative multiplication, their multi-linear symmetry has to be taken into account in order to achieve correct simplifications of expressions like the fifth derivative

$$y^v = f'''' \cdot f \cdot f \cdot f \cdot f + 6f''' \cdot f' \cdot f \cdot f \cdot f + 4f'' \cdot f'' \cdot f \cdot f \cdot f + 4f'' \cdot f'^2 \cdot f \cdot f +$$
$$+ 3f'' \cdot f' \cdot f \cdot f' \cdot f + f' \cdot f''' \cdot f \cdot f \cdot f + 3f' \cdot f'' \cdot f' \cdot f \cdot f + f'^2 \cdot f'' \cdot f \cdot f + f'^4 \cdot f .$$

(I hope I've gotten it right.)

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The foregoing *formal* (because their convergence is undetermined) Taylor series expansions do not reveal an important property possessed by the computed solution Y of the Initial Value Problem when it is obtained from a *Reflexive* formula, which is a formula in which Y(t+h) and y(t) are merely swapped when the sign of h is reversed. The Midpoint and Trapezoidal Rules' formulas are reflexive. The composition of T/h steps of a reflexive formula to approximate the true solution y(T) at a fixed T , but using any sufficiently small stepsize h so long as T/h is an integer, can be proved to produce a computed approximation Y(T) that depends upon h and differs from y(T) by an error

$$y(T) - Y(T) = c_2h^2 + c_4h^4 + c_6h^6 + \dots$$

whose formal expansion in powers of h contains only even powers. The expansion need not converge for any $h > 0$; instead it is an *Asymptotic* expansion whose behavior is conveyed by its first few terms ever more accurately as $h \to 0$. Recomputations of Y(T) with diminishing stepsizes h, h/2, h/4, h/8, … provides a sequence to which *Richardson's Extrapolation* can be applied, as in *Romberg* integration, to achieve what amounts to higher-order convergence.