Taylor expansion methods for solving ODEs

Inefficient version: Repeated differentiation; described in many text books. However useful in the context of deriving Runge-Kutta formulas.

Given $y' = f(t,y)$; by repeated differentiation:

$$y'' = f\frac{\partial f}{\partial y} + \frac{\partial f}{\partial t},$$

$$y''' = f^2\frac{\partial^2 f}{\partial y^2} + f\left\{2\frac{\partial^2 f}{\partial t\partial y} + \left(\frac{\partial f}{\partial y}\right)^2\right\} + \frac{\partial f}{\partial t}\cdot\frac{\partial f}{\partial y} + \frac{\partial^2 f}{\partial t^2},$$

$$y'''' = f^3\frac{\partial^3 f}{\partial y^3} + f^2\left\{3f\frac{\partial^3 f}{\partial t\partial y^2} + 4\frac{\partial f}{\partial y}\cdot\frac{\partial^2 f}{\partial y^2}\right\} + \frac{\partial f}{\partial t}\cdot\left(\frac{\partial f}{\partial y}\right)^2 + \frac{\partial^3 f}{\partial t^3} + 3\frac{\partial f}{\partial t}\cdot\frac{\partial^2 f}{\partial t\partial y} + \frac{\partial^2 f}{\partial t^2}\cdot\frac{\partial f}{\partial y} +$$

$$+ f\left\{\left(\frac{\partial f}{\partial y}\right)^3 + 5\frac{\partial^2 f}{\partial t\partial y}\cdot\frac{\partial f}{\partial y} + 3\frac{\partial^3 f}{\partial t^2\partial y} + 3\frac{\partial f}{\partial t}\cdot\frac{\partial^2 f}{\partial y^2}\right\}$$

... etc. (a big mess to find many terms in this way)

Knowing $y(t_i)$, we can compute

$$y(t_{i+1}) = y(t_i + k) = y(t_i) + k\, y'(t_i) + \frac{k^2}{2}y''(t_i) + \frac{k^3}{6}y'''(t_i) + \ldots \tag{1}$$

and then choose *k* so that the last used term is safely below the desired local error level; repeat at t_{i+1}, etc., and proceed (using variable step size, if needed) from initial to final time.

Somewhat more efficient version: Recursive calculation of expansion coefficients.

Given a value for *y* at time *t*, we choose some desired local order *n* and then want to generate the coefficients in the exact counterpart to (1)

$$y(t+k) = y(t) + a_1 k + a_2 k^2 + a_3 k^3 + \ldots + a_n k^n + O(k^{n+1}). \tag{2}$$

As an example, we choose $f(t,y) = t^2 + y^2$, i.e. the ODE is

$$y' = t^2 + y^2 \ . \tag{3}$$

The expansion (2) is now obtained by the Mathematica script

```
n=8;                                 (* Specify number of coefficients *)
y[k_]:=y+Sum[aᵢkⁱ,{i,1,n}]+O[k]ⁿ⁺¹; (* Taylor expansion with unknown coef.*)
f[t_,y_]:=t²+y²;                     (* Specify the RHS of the ODE *)
LogicalExpand[y'[k]==f[t+k,y[k]]  (* Create the coefficient relations *)
```

which produces the output

$t^2+y^2-a_1==0\&\&2t+2y\ a_1-2a_2==0\&\&1+a_1^2+2y\ a_2-3a_3==0\&\&$
$2a_1a_2+2y\ a_3-4a_4==0\&\&a_2^2+2a_1a_3+2y\ a_4-5a_5==0\&\&2a_2a_3+2a_1a_4+2y\ a_5-6a_6==0\&\&$
$a_3^2+2a_2a_4+2a_1a^5+2y\ a_6-7a_7==0\&\&2a_3a_4+2a_2a_5+2a_1a_6+2y\ a_7-8a_8==0$

A lot more efficient version:

Start by considering the ODE in the form

$$\frac{dy(t+k)}{dk}=f(t+k,y(t+k)). \tag{4}$$

Each time a truncated expansion (2) is substituted into the THS of (4), re-expanded in powers of *k* and then integrated with respect to *k*, we gain one more correct coefficient in the expansion (2). By starting with our initial condition (at *t*), and truncating so we never include any more terms than what we know to be correct, the algebra remains very moderate, and we might not even need any symbolic package (such as Mathematica) to generate a sequence of coefficients.

An extremely efficient continued fraction (Padé) generalization:

The recursive Taylor series method (described just above) can be improved further by, at each time step, convert the generated Taylor expansion to Padé rational form before it is actually numerically evaluated. This makes it possible to integrate straight through low order poles (which cause virtually all other ODE solvers to fail) or to pass nearby such singularities (which might be located in the complex plane near the path of integration) without loss of efficiency.

In the ODE (3) we considered above, with initial condition $y(0)=0$, there is an analytic solution available: $y(t)=t\frac{J_{3/4}(t^2/2)}{J_{-1/4}(t^2/2)}$, see Figure 1.

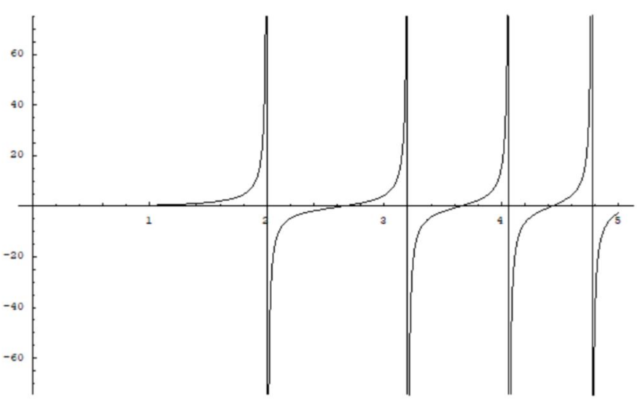

Figure 1. The function $y(t)=t\frac{J_{3/4}(t^2/2)}{J_{-1/4}(t^2/2)}$ displayed over the interval $0\le t\le 5$.

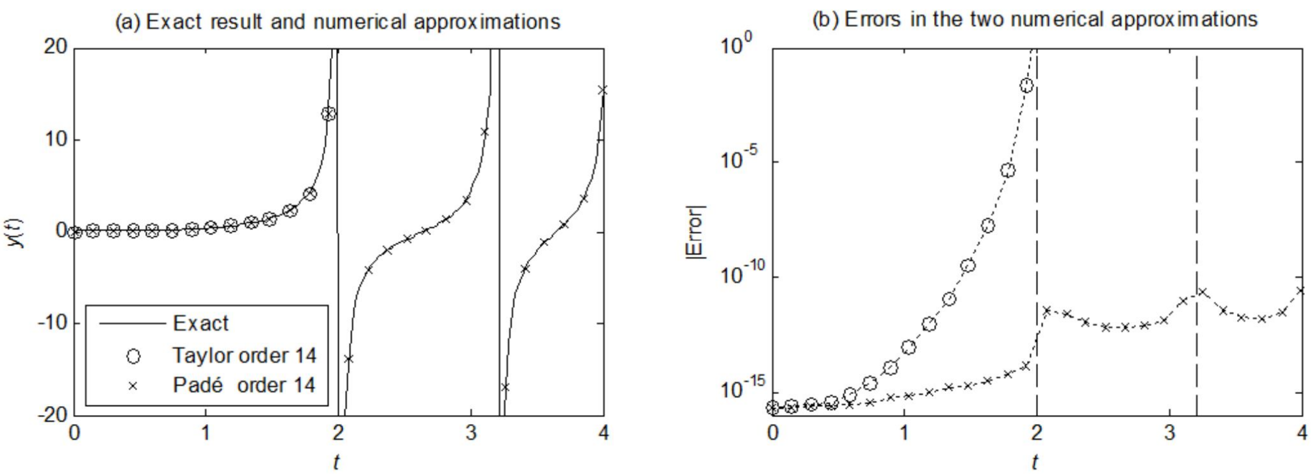

Figure 2. Comparison between the original Taylor series method and this Padé enhancement when solving (1), expanding to 14 Taylor terms, using steps of size $k = 4/27 \approx 0.15$ (figure copied from [3]).

Already the Taylor series method is spectacularly accurate when the pole is approached, given the coarse step size that is used. With the Padé enhancement, there is some loss of accuracy very near to a pole, since the calculation involves subtractions of large numbers to generate small numbers. With slight precautions, it is possible to numerically integrate accurately vast distances through pole fields.

Some relevant references:

[1] D. Barton, I.M. Willers and R.V.M. Zahar, An implementation of the Taylor series method for ordinary differential equations, *Comp. J.* 14 (1971), 243-248.

[2] G. Corliss and Y.F. Chang, Solving ordinary differential equations using Taylor series, *ACM Trans. Math. Software*, 8 (1982), 114-144.

[3] B. Fornberg and J.A.C. Weideman, A numerical methodology for the Painlevé equations, *J. Comput. Phys.* 230 (2011), 5957-5973.

[4] E. Hairer, S.P. Nørsett and G. Wanner, Solving Ordinary Differential Equations I – Non-Stiff Problems, Springer Verlag, Berlin, 1987. See especially pp. 45-47.

[5] I.M. Willers, A new integration algorithm for ordinary differential equations based on continued fraction approximation, *Comm. of the ACM*, 17 (1974), 504-508.