Numerical integration of Cauchy problems with singular points

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Abstract. Detection and investigation of moving singular points in solutions of differential equations is traditionally performed using computer algebra systems. We propose a number of approaches to solve this problem in the framework of finite-difference methods. Algorithms are described that permit to calculate of the singularity position and order and to continue the solution through a sequence of integer order poles.

Introduction

Singularity occurrence is a considerable difficulty for numerical integration of Cauchy problem for ordinary differential equations (ODEs). Commonly, the singularity position is unknown a priori. Euler noticed that as one approaches the singularities of the Riccati equation, the approximate solution diverges from the exact one. Therefore, computer algebra methods are widely used to study singularities.

The problem of completely numerical detection and investigation of singularities in Cauchy problem solutions was stated by Marchuk at his seminar at the Institute of Computational Mathematics of the Russian Academy of Sciences in 2003. The methods described in the present work can be easily generalized to the case of ODE systems, but for simplicity, we consider the problem in scalar formulation. For the ODE

$$du/dt = f(u, t), \tag{1}$$

the aim is to detect the nearest moving singular point, determine its type, and calculate the moment of the singularity occurrence and its order with guaranteed accuracy. The pioneer work of Alshina, Kalitkin and Koryakin [1] proposed to detect a singularity by a sharp drop in the effective order of accuracy at the moment of reaching the singularity. Cauchy problems with multiple poles have traditionally been considered for the Painlevet transcendentals, for which there is a lot of a priori information. General numerical methods for such problems have not been developed.

In this paper, we propose an improved procedure for detecting the nearest singularity, based on selection of arc length of the integral curve as new integration argument. This significantly improves accuracy and robustness of diagnostics and even perform it in automatically. For problems with multiple poles of the integer order $q \geq 1$, we propose a method of through calculation of Cauchy problems.

1. Detection of the nearest singularity

In (1), let us select the arc length of the integral curve $dl^2 = dt^2 + du^2$ as new integration argument [2]. Thereby, time t also becomes an unknown function and the dimension of the problem increases by one. In the new argument, the system takes the form

$$du/dl = f(1+f^2)^{-1/2}, \quad dt/dl = (1+f^2)^{-1/2}. \tag{2}$$

This technique has two advantages. Firstly, the vector of right-hand parts of the system (2) has unit length. This greatly simplifies numerical calculation. Secondly, the singularity $u \to \infty$ corresponds to infinite arc length $l \to \infty$. Therefore, for calculation up to some finite l, the singularity does not fall inside the integration segment. Let us calculate the problem (2) according to some numerical scheme of order of accuracy p on a mesh with step h and find the numerical solution t_n, u_n.

Let the nearest singular point T of the function $u(t)$ be algebraic. Then the decomposition $u = C(T-t)^{-q} + \ldots$ holds in its neighborhood. Differentiating this relation, one gets $f = qu/(T-t)$. Writing the last equality in the nodes n and $n+1$, one obtains one-step formulas for determining q and T

$$q_{n+1} = (t_{n+1} - t_n)(u_n/f_n - u_{n+1}/f_{n+1})^{-1}, \quad T_{n+1} = qu_n/f_n + t_n. \tag{3}$$

If during calculation, the values q_{n+1} and T_{n+1} tend to some limits, then the behavior of the solution is determined by the first term of the Puiseux series, and the singular point can be reliably determined. Similarly, one can detect singularities of the form $\ln^q(T-t)$ and $(T-t)^{-q}\ln(T-t)$.

Next, let us perform similar calculations on a mesh with steps $h/2$. Even nodes of this mesh exactly coincide with the previous mesh with steps h. Comparing solutions in coinciding nodes, let us find error estimates of the solution and the singularity parameters by the Richardson method [3]

$$\Delta u = D(u_h - u_{h/2}),\ \Delta q = D(q_h - q_{h/2}),\ \Delta T = D(T_h - T_{h/2}),\ D = (2^p - 1)^{-1}. \tag{4}$$

These estimates are asymptotically sharp. Practically, they are indistinguishable from the real error equal to the difference between the exact and numerical solutions.

The proposed method has been verified on a number of test problems with known exact solutions, including partial differential equations. Among them, the

S-mode of nonlinear combustion $u_t = (u^2 u_x)_x + u^3$ has been considered. Via the method of lines, this equation is reduced to a system of several hundred ODEs

$$du_j/dt = (2h_x^2)^{-1}\left[(u_{j+1}^2 + u_j^2)(u_{j+1} - u_j) - (u_j^2 + u_{j-1}^2)(u_j - u_{j-1})\right] + u_j^3. \quad (5)$$

Here j and h_x are spatial node number and the space value, respectively. In the performed tests, it was possible to determine T with the accuracy of round-off errors $10^{-8} \div 10^{-10}$.

2. Pole sequence

Let us describe an algorithm for integrating the Cauchy problem, the solution of which has a sequence of poles. Consider the so-called reciprocal function $v = \mathrm{sgn}(u)|u|^{-1/q}$. It satisfies the differential equation

$$dv/dt = -q^{-1} v^{1+q} f(v^{-q}). \quad (6)$$

If u has a pole of order q at a point T, then v has a prime zero at that point. Calculating such a zero is of no difficulty.

Let us introduce a mesh in the time argument with step of τ and calculate the problem (1) according to some scheme of the order of accuracy p. Simultaneously, let us calculate q_{n+1} and T_{n+1} using the formulas (3). Naturally, the calculated values of q_{n+1} are non-integer. However, if during several sequential steps, they are close to some integer q, then the latter can be considered the order of the nearest pole. This calculation is performed until the condition $u_n > U$ is met for the mesh value u_n, where U is a threshold value. Denote this node number by n^*. Beyond this point, let us numerically solve the problem (6) on the same mesh with initial condition $v_{n^*} = 1/u_{n^*}$. Simultaneously, in all subsequent mesh nodes, we restore the numerical value of $u(t)$ by $u_n = 1/v_n$.

Change of sign of v_n implies zero of the function $v(t)$ which corresponds to pole of the function $u(t)$. Thereby, one finds the solution on both sides of the pole and can continue the calculation through the pole. Further, if solution of (6) meets the condition $|v_n| > 1/U$, then one returns to the solution of (1). This transition can be performed an unlimited number of times. This method allows for calculation through a pole or a sequence of poles.

Note that in this method, one can also apply the arc length of the integral curve as an argument. This increases robustness of the algorithm. For the functions $u(t)$ and $v(t)$, the integral curves are different, accordingly, the arc length for them is also different. Therefore, the starting point of the arc length should be in the transition point each time.

The reciprocal function method has been tested on the Riccati equation with the exact solution $u = u_0 + \mathrm{tg}\, t$ including first-order poles, and on a specially constructed autonomous equation with the exact solution $u = u_0 + \mathrm{tg}^3(t - t_0) + \mathrm{tg}(t - t_0)$ containing third-order poles. Test calculations have shown that solution with multiple poles can be calculated even using explicit Runge-Kutta schemes and get an accuracy of 10^{-14}, comparable to round-off errors.

3. Proximity of curves

In problems with singularities, error calculation as a traditional norm (C, L_2, or similar) of difference between the the numerical and the exact solutions is non-constructive. The reason is that the calculated position of the pole differs from the exact one, and therefore, formal solution difference near the pole is huge.

We propose to use the Hausdorff metric to estimate the proximity of solutions. Let us describe the procedure for calculating it. Consider the exact solution $u(t)$ before the first pole or between two adjacent poles. Consider the mesh solution u_n relating to the mentioned section of the exact solution; it consists of points with coordinates (t_n, u_n). Some of the values of u_n are calculated directly by solving the equation (1), and the values lying near the poles are restored from calculated values of v_n. Draw perpendicular from each point (t_n, u_n) to the curve $u(t)$. The length of this perpendicular d_n is the distance from the point to the curve. Taking $d = \ max d_n$, one gets the Hausdorff metric, which is similar to the C norm. In practice, it is more convenient to use the analog of the L_2 norm, which is equal to the root mean square of d_n

$$d^2 = N^{-1} \sum\nolimits_{n=1}^{N} d_n^2, \tag{7}$$

where N is the total number of points in the selected section. For example, for calculation of the Riccati equation via the 2nd order Runge-Kutta scheme with step $\tau = 0.003$, the value d was 10^{-4}, however, there was no proximity in the L_2 norm.

Conclusion

We show that the classical problem of determining moving singularities allows for a purely numerical solution. The parameters of the singularity can be calculated with the accuracy of computer round-off errors. The method of detecting the nearest singularity is implemented as a package in the MatLab environment. It works in a completely automatic (not interactive!) mode. The package is tested on representative problems, including partial differential equations. A detailed description of the results of this work is given in [4, 5].

References

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