Validated Explicit and Implicit Runge-Kutta Methods[1]

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Introduction

The guaranteed solution of initial value problem of ordinary differential equations is well studied from interval analysis community. In the most of the cases Taylor models are used in this context, see [1] and the references therein. In contrast, in numerical analysis community other numerical integration methods, e.g., Runge-Kutta methods, are used. Indeed, these methods have very good stability properties [2] and they can be applied on a wide variety of problems.

We propose a new method to validate the solution of initial value problem of ordinary differential equations based on Runge-Kutta methods. The strength of our contribution is to adapt any explicit and implicit Runge-Kutta methods to make them guaranteed. We experimentally verify our approach against Vericomp benchmark[2] and the results are reported in [3]. We hence extend our previous work [5] on explicit Runge-Kutta methods.

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[2]http://vericomp.inf.uni-due.de, we consider results dated back to October 2014.

Main idea

We want to solve

$$\dot{\mathbf{x}}(t) = f(t, \mathbf{x}(t)) \quad \text{with} \quad \mathbf{x}(0) = \mathbf{x}_0 \ . \tag{1}$$

We denote by $\mathbf{x}(t; \mathbf{x}_0)$ the solution of Equation (1) at a time t associated to the initial value $\mathbf{x}_0$. Applying a s-stage Runge-Kutta method on Equation (1), we have the following recurrence relation

$$k_i = f\left(t_n + c_i h_n, \mathbf{x}_n + h \sum_{j=1}^{s} a_{ij} k_j\right), \qquad \mathbf{x}_{n+1} = \mathbf{x}_n + h \sum_{i=1}^{s} b_i k_i \ .$$

The coefficients c_i, b_i and a_{ij} with $i, j = 1, 2, \ldots, s$ are associated to a given Runge-Kutta methods, see [2] for more details. That is for each time instant t_n, we have $\mathbf{x}_n \approx \mathbf{x}(t_n; \mathbf{x}_{n-1})$.

The challenge to make Runge-Kutta guaranteed is to compute a safe bound of the local truncation error (LTE for short) at each time t_n, that is $\mathbf{x}(t_n; \mathbf{x}_{n-1}) - \mathbf{x}_n$ must be bounded. An elegant solution to compute the formula of the LTE is based on the order condition of Runge-Kutta methods. A Runge-Kutta method has order p, i.e., $\mathbf{x}(t; \mathbf{x}_{n-1}) - \mathbf{x}_n \leq C \cdot \mathcal{O}(h^{p+1})$, with C a constant independent of f, if and only if the Taylor expansion of the true solution and that of the numerical solution have the same coefficients for the $p + 1$ first terms. In consequence, the formula of the LTE of a Runge-Kutta methods is given by the difference of the remainders of the two Taylor expansions.

Main results

John Butcher in [4] defines a generic method to compute the Taylor expansion of the true and a numerical solutions of Equation (1). It is based on the Fréchêt derivatives F of the function $\mathbf{x}(t)$. The great idea of John Butcher is to connect these Fréchêt derivatives of a given order m to a combinatorial problem to enumerate the number of trees τ with q nodes.

In summary, in [4] we have

$$\mathbf{x}^{(q)}(t) = \sum_{r(\tau)=q} \alpha(\tau) F(\tau), \quad \text{and} \quad \mathbf{x}_n^{(q)} = \sum_{r(\tau)=q} \alpha(\tau)\gamma(\tau)\psi(\tau)F(\tau) \ .$$

with $\mathbf{x}^{(q)}(t)$ the q-th time derivative of the true solution and $\mathbf{x}_n^{(q)}$ the q-th time derivative of the numerical solution of Equation (1). Coefficients $\alpha(\tau)$ and $\gamma(\tau)$ are characteristics of trees τ, see [4] for more details. Note that the coefficient $\psi(\tau)$ is a function of the coefficients c_i, b_i and a_{ij}, $i = 1, 2, \cdots, s$.

Using the approach of John Butcher, we can validate any Runge-Kutta methods of order p using the following expression of the LTE

$$\text{LTE}(t, \mathbf{x}(\xi)) = \frac{h^{p+1}}{(p+1)!} \sum_{r(\tau)=q} \alpha(\tau)[1 - \gamma(\tau)\psi(\tau)]F(\tau)\,(\mathbf{x}(\xi)) \quad \text{with} \quad \xi \in]t_n, t_{n+1}[\ .$$

Using a classical 2-step approach of guaranteed integration, see [1], from a given guaranteed initial value $[\mathbf{x}_n]$ at time instant t_n then

1. compute an enclosure $[\tilde{\mathbf{x}}]$ of $\mathbf{x}(t)$ on the time interval $[t_n, t_{n+1}]$;
2. compute a tight enclosure of the solution $[\mathbf{x}_{n+1}]$ at time t_{n+1} using Runge-Kutta method and the LTE formula with $[\tilde{\mathbf{x}}]$.

In summary, our approach is defined by

$$k_i(t, \mathbf{x}_n) = f\left(t_j + c_i(t - t_j), \mathbf{x}_n + (t - t_n)\sum_{j=1}^{s} a_{ij}k_j\right), \tag{2a}$$

$$\mathbf{x}_{n+1}(t, \xi) = \mathbf{x}_n + (t - t_n)\sum_{i=1}^{s} b_i k_i(t, \mathbf{x}_n) + \text{LTE}(t, \mathbf{x}(\xi)) \ . \tag{2b}$$

Equation (2) can be used for computing a priori enclosure and tightening the solution. Note that in case of implicit Runge-Kutta methods, the equations k_i, for $i = 1, \ldots, s$, form a contracting system of equations. In consequence, we can easily build an interval contractor from the system of k_i and so we can solve it easily.

To illustrate our approach, we consider Vericomp Problem 61

$$\begin{cases} \dot{x}_1 = 1, & x_1(0) = 0 \\ \dot{x}_2 = x_3, & x_2(0) = 0 \\ \dot{x}_3 = \frac{1}{6}x_2^3 - x_2 + 2\sin(p \cdot x_1) \quad \text{with} \quad p \in [2.78, 2.79], & x_3(0) = 0 \ . \end{cases}$$

Using a validated version, with our approach, of Lobatto-3C implicit Runge-Kutta method of order 4, we obtain 10.597 as the maximal width of the solution enclosure at 10 seconds (tolerance 10^{-10} on LTE) while none of Riot, Valencia-IVP, nor VNODE-LP can produce a solution at 10 seconds.

Conclusion

We presented a new class of validated numerical integration method based on explicit and implicit Runge-Kutta methods. We have a generic formula to compute the LTE. We show that our approach has the ability to solve problems that state-of-the art methods cannot.

References

[1] N. S. Nedialkov, K. R. Jackson, and G. F. Corliss, Validated solutions of IVPs for ordinary differential equations, *Applied Mathematics and Computation*, 105(1):21 – 68, 1999.

[2] E. Hairer, S. Norsett, and G. Wanner, *Solving Ordinary Differential Equations I: Nonstiff Problems*, Springer-Verlag, 1993.

[3] J. Alexandre dit Sandretto and A. Chapoutot, Validated Solution of IVP for ODE based on Explicit and Implicit Runge-Kutta Schemes, *Research report ENSTA ParisTech*, 2015.

[4] J. C. Butcher, Coefficients for the study of Runge-Kutta integration processes, *Journal of the Australian Mathematical Society*, 3:185–201, 1963.

[5] O. Bouissou, A. Chapoutot and A. Djoudi, Enclosing Temporal Evolution of Dynamical Systems Using Numerical Methods, *NASA Formal Methods*, LNCS volume 7871, Springer Verlag, 2013.