Evaluation of the Communications in Applied Mathematics and Computational Science submission

Positivity-Preserving Adaptive Runge Kutta Methods

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Summary:

This manuscript studies the efficiency of a new kind of Positivity-Preserving Runge-Kutta Methods. The main idea in the new approach consists in adaptively choosing the weights b of the RKM in a way that ensures positivity, or other bound constraints, for problems satisfying the sufficient condition (1.4). One of the main benefits of this new approach is that all linear invariants of the problem are preserved. Other projection methods also preserve invariants, but only if you explicitly know these invariants. If any component of the numerical solution is negative, a linear program (LP) must be solved at each step in order to choose the new weights, and this could be an extra time consuming process. Nevertheless, the idea of minimizing the deviation of the weights is simple and in some cases may be much more efficient, particularly for large systems. The numerical experiments are well presented and quite thorough including different stiff and non-stiff problems, with fixed and adaptive step size implementations.

Comments:

Positivity-Preserving methods have been studied quite a lot in recent decades and the authors have summarized really well the state of art in the introduction by referring to Projection methods, SSPRK methods, MPRK methods and DSRK positive methods. In the new schemes proposed the weights of some baseline RKM are adapted in order to ensure positivity or other bounds. These new methods are valid both for stiff and non-stiff problems satisfying the sufficient condition for positivity (1.4). In addition, the authors clarify that for some positive problems not satisfying (1.4) numerical tests did not show promising results. I personally value the algorithm given in Section 3. Theorem 4.1 about the stability region of the new adaptive Runge-Kutta method with convex adaptation is quite interesting, particularly for A-stable methods. Lemma 4.2 with the bound for the stability function of the adapted method is interesting too. The paper is clear and well written, thus I would recommend this work to be published provided that the authors address properly the points listed below.

2. **Bound-preserving adaptive Runge–Kutta methods**

   (a) In equation (2.14b), it is weird to read $-0.01u_2$ and $-0.05u_2$ in the same line. Is it an error? The same thing happens in equations (2.14c) with u_3, in (5.5b) with u_2, and in (5.5c) with u_3.

   (b) In Figure 1, in the difference $\|\tilde{b} - b\|_1$, a tilde is missing.

3. **Selection of the modified weights**

   (a) In section 3.2, two different approaches to adapt the weights are considered: Free adaptation and Convex adaptation. At the same time, it is explained that "...we can additionally impose either or both of the following strategies:

      1. Select in advance a set of desirable weight vectors b^1, $b^2, \ldots$
      2. Require that the perturbation $\|\tilde{u} - u\|$ is small ..."

I think that the first strategy is nothing but the second approach (Convex adaptation). I suggest making this part clearer in order to avoid confusion between approaches and strategies.

4. **Properties of adaptive RKMs**

   (a) Figure 3a, with free adaptation of the weights $\tilde{b}$, does not give enough information about the stability regions of the adapted methods. In my opinion, it would be clearer if each stability curve was labeled with the value of the difference $\|\tilde{b} - b\|_1$, accordingly with the values in Figure 4b. In this way we could see the progress of the stability regions during the numerical integration process.

   (b) In the first line of formula (4.6) the vector $(\tilde{b} - b)$ should be $(\tilde{b} - b)^T$.

5. **Numerical experiments**

   (a) In the third line of Section 5.1, RHS appears for the first time without explaining its meaning.

   (b) In section 5.1, just before the formula (5.1), it is said "Since the positivity of the stage values is not ensured, the right hand side has to be defined for negative values. If this is not the case, the right hand side has to to be adapted accordingly". This is a bit confusing, particularly the text "...has to be defined for negative values...". I suggest that you make this part clearer.

   (c) In formula (5.2), the last u_{i-1}, shouldn't it be u_i?

   (d) After formula (5.2) "...In Figure 4a the results for $\Delta t = 0.015$ are plotted for different time steps..." should be "...In Figure 4a the results for $\Delta t = 0.015$ are plotted for different values of time t..."

   (e) Figure 5, about the non-stiff problem with fixed stepsize, is quite interesting and gives information about the convergence of the adapted mehtod. For $\Delta t = 0.0082$ the unaltered method leads to positive solutions. For $\Delta t = 0.015$ the original method leads to negative values in the interval $[0, 0.375]$ and the weights are altered by solving an LP problem. Is this extra time consuming a significant cost or could it be an economical alternative to using excessively small step sizes? A further explanation about this issue should be added.

   (f) In Figures 6c and 6d, in the difference $\|\tilde{b} - b\|_1$ and also in the legend, a tilde is missing.

   (g) In the third subplot of Figure 9, in the difference $\|\tilde{b} - b\|_1$, a tilde is missing.

   (h) In the fourth subplot of Figure 11, in the difference $\|\tilde{b} - b\|_1$, a tilde is missing.