Presentation, error analysis and numerical experiments on a group of 1-step-ahead numerical differentiation formulas

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In order to achieve higher computational precision in approximating the first-order derivative of the target point, the 1-step-ahead numerical differentiation formulas are presented. These formulas greatly remedy some intrinsic weaknesses of the backward numerical differentiation formulas, and overcome the limitation of the central numerical differentiation formulas. In addition, a group of formulas are proposed to obtain the optimal step length. Moreover, the error analysis of the 1-step-ahead numerical differentiation formulas and the backward numerical differentiation formulas is further investigated. Numerical studies show that the proposed optimal step-length formulas are effective, and the performance of the 1-step-ahead numerical differentiation formulas is much better than that of the backward numerical differentiation formulas in the first-order derivative approximation.

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1. Introduction

Numerical differentiation, which is usually used to solve ordinary differential equations (ODEs) and partial differential equations (PDEs) [1–5], has been widely applied in numerical analysis [5,6] and engineering applications [7–9]. With discrete sampling points of the given target function, different methods can be used to obtain the approximation of the first-order derivative at the target point, such as the polynomial interpolation method, the finite difference method, the regularization method and the method of undetermined coefficients [10]. However, considering the following two situations: (1) that the backward differentiation formulas may not adapt to the fast variational rate of the first-order derivative of target point, and (2) that the central differentiation formulas cannot approximate the first-order derivative of the target points without enough number of data points on either side, a new kind of 1-step-ahead numerical differentiation formulas is needed.

In addition, it is an important task in the numerical differentiation to analyze the total errors of such 1-step-ahead numerical differentiation formulas. Here, the total errors contain two parts, i.e., the round-off errors and the truncation errors. Besides, from the previous work [5], we know that the step length brings about a great influence on the total errors. Thus, in this paper, we will mainly investigate the relationship between the step length and the total error, and, finally, analyze and find out the optimal step length to minimize the total error. Lots of numerical experimental results indicate that the optimal step-length formulas are effective.

The remainders of this paper are organized into four sections and two appendices. In Section 2, the 1-step-ahead numerical differentiation formulas using two to seven data points are presented. In Section 3, the total errors are analyzed and the related numerical experimental results are illustrated. The comparison of the errors between the presented 1-step-ahead numerical differentiation formulas and the backward numerical differentiation formulas is further discussed in Section 4, and conclusions are in Section 5. In Appendix A, we present a novel method as the proof of the related formula,