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Output error estimation for summation-by-parts finite-difference schemes ☆

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ABSTRACT

The paper develops a posteriori error estimates of integral output functionals for summation-by-parts finite-difference methods. The error estimates are based on the adjoint-weighted residual method and take advantage of a variational interpretation of summation-by-parts discretizations. The estimates are computed on a fixed grid and do not require an embedded grid or explicit interpolation operators. For smooth boundary-value problems containing first and second derivatives the error estimates converge to the exact error as the mesh is refined. The theory is verified using linear boundary-value problems and the Euler equations.

1. Introduction

Integral functionals that depend on the solution of a partial differential equation arise in many fields of science and engineering; an example from fluid mechanics is the drag force on a body immersed in a flow. Indeed, approximating a functional (or functionals) is frequently the motivation for numerically solving a partial differential equation. In such circumstances, estimating the error in the output functional is of great value to assess the predictive value of the simulations.

Around the turn of the twenty-first century, several authors began exploring the use of the adjoint variables for a posteriori output error estimation [1–5]. This adjoint-weighted residual method has proven to be highly effective for both output error estimation and mesh adaptation; see [6] for a recent review in the context of computational fluid dynamics (CFD).

This paper presents a formulation of the adjoint-weighted residual method for summation-by-parts (SBP) finite difference methods. SBP operators are high-order finite-difference operators that respect a discrete version of integration by parts [7] that leads to attractive stability properties. SBP operators have been used successfully in a number of fields, including CFD [8–12] and general relativity [13,14].

In addition to stability, the SBP definition has important consequences for functional accuracy. In [15] it was shown that diagonal-norm SBP operators produce approximate functionals that are superconvergent relative to solution accuracy. In the present work, we will see that SBP discretizations are high-order approximations to the variational form of boundary value problems. This variational interpretation of SBP discretizations plays an important role in our theory of error estimates for integral functionals.

The proposed output error estimates, while based on the well-established adjoint-weighted residual method, have some unique characteristics compared with existing approaches developed for finite-element and finite-volume discretizations. Most significantly, SBP error estimates are constructed on a fixed grid with a fixed number of degrees of freedom. This

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differs from finite-volume approaches that use embedded grids or finite-element methods that use p enrichment. SBP error estimates are formed by approximating the residual error using existing higher-order SBP operators; these operators define a high-order reconstruction that does not require an explicit interpolation of the solution or adjoint. Moreover, while a higher-order SBP operator is needed to approximate the residual error, a higher-order solution or adjoint is not needed.

The content of the paper is organized as follows. Section 2 reviews SBP operators and discusses the variational interpretation of SBP discretizations. Section 3 develops the theory of SBP output-error estimates for a model advection problem; subsequently, we discuss how the theory can be extended to more general problems and how the estimates are implemented. The theory is verified using numerical examples in Section 4. The examples include two-dimensional linear problems and flows described by the Euler equations. Conclusions and future work are summarized in Section 5.

2. SBP discretizations: notation and background

Let the domain $\Omega = [0,1]$ be discretized using $n+1$ uniformly spaced points $x_k = kh$, $k = 0,1,\ldots,n$, with mesh spacing $h = 1/n$. We will assume domains other than $[0,1]$ can be mapped to Ω using a sufficiently differentiable transformation, i.e. a transformation whose smoothness is consistent with the finite-difference operators employed. Further details regarding more general domains and grids can be found in Section 3.3.2.

Capital letters with a script type denote functions from an appropriate inner-product space on the domain Ω. For example, $\mathcal{U}(x) \in C^p[0,1]$ is a function from the set of p-times differentiable functions that are square integrable on the interval $[0,1]$. Small roman letters in a serif type indicate a function restricted to the grid. This restriction operation is illustrated below using $\mathcal{U}(x)$ and $u \in \mathbb{R}^{n+1}$.

$$u = [\mathcal{U}(x_0) \quad \mathcal{U}(x_1) \quad \cdots \quad \mathcal{U}(x_n)]^T.$$

A vector with subscript h, e.g. $u_h \in \mathbb{R}^{n+1}$, indicates that the vector is the solution of a difference equation on a grid with spacing h.

The first and last columns of the $(n+1) \times (n+1)$ identity matrix frequently appear when manipulating SBP operators. We will denote these columns by the unit vectors $e_0, e_n \in \mathbb{R}^{n+1}$:

$$e_0 = [1 \quad 0 \quad 0 \quad \cdots \quad 0 \quad 0]^T,$$
$$e_n = [0 \quad 0 \quad 0 \quad \cdots \quad 0 \quad 1]^T.$$

The following rank-one matrices based on e_0 and e_n will also prove useful:

$$e_0\, e_0^T = \text{diag}\ (1,0,0,\ldots,0) \quad \text{and} \quad e_n\, e_n^T = \text{diag}\ (0,0,\ldots,0,1).$$

We use order notation as a shorthand to indicate bounds on various terms. Specifically, we write $F(h) = \mathrm{O}(h^p)$ if and only if $\exists M > 0$ and $h_\star > 0$ such that

$$|F(h)| \leqslant Mh^p, \quad \forall\ h < h_\star.$$

2.1. Summation-by-parts operators

The summation-by-parts (SBP) property refers to a discrete analog of integration-by-parts. The SBP property is useful because it can establish the linear time-stability of a semi-discrete scheme. This was partly the motivation given by Kreiss and Scherer [7] when they first proposed high-order finite-difference methods that obey the SBP property; see also [16].

This work focuses on discretizations involving diagonal-norm SBP operators; therefore, the formal definition below is restricted to this type of first-derivative operator. However, the results can be extended to SBP operators with more general norms (e.g. the so-called full and restricted-full norms).

Definition 1 (*Diagonal-norm summation-by-parts operator*). The matrix $D_p \in \mathbb{R}^{(n+1)\times(n+1)}$ is a summation-by-parts operator for the first derivative if it has the form

$$D_p = H_p^{-1} Q_p,$$

where $H_p \in \mathbb{R}^{(n+1)\times(n+1)}$ is a diagonal weight matrix with strictly positive entries $H_{ii} = \mathrm{O}(h)$, and $Q_p \in \mathbb{R}^{(n+1)\times(n+1)}$ satisfies

$$Q_p + Q_p^T = \text{diag}\ (-1,0,0,\ldots,0,1) = e_n\, e_n^T - e_0\, e_0^T.$$

Furthermore, D_p is a $2p$-order-accurate approximation to d/dx at the interior nodes, $\{x_k | 2p \leqslant k \leqslant n-2p\}$, and a p-order-accurate approximation at the boundary nodes, $\{x_k | 0 \leqslant k \leqslant 2p-1\}$ and $\{x_k | n-2p+1 \leqslant k \leqslant n\}$.