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Laguerre and Hermite Collocation Methods for Unbounded Domains

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Abstract. We discuss spectral collocation methods based on Jacobi-Gauss-Lobatto points and Laguerre and Hermite collocation for unbounded domains. These methods are well conditioned, and some numerical experiments demonstrate quite high accuracy.

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Key words: Collocation method, condition number, stability.

1. Introduction

The spectral collocation method that we consider approximates derivatives by direct differentiation of Lagrange interpolation polynomials at Gauss-type points. In applications involving non-linear problems or equations with variable coefficients, the performance of this approach is comparable to high-order finite difference methods and superior to the spectral method with modal basis functions. Nevertheless, it involves ill-conditioned linear systems when direct solvers and iteration methods exploiting a large number of collocation points are used. Various approaches to address this issue have been discussed. Coutsias and others [4, 5, 8, 16] proposed the integration preconditioning method, and Greengard [9] and El-Gendi [7] considered the spectral integration method. Wang *et al.* [23] introduced a Legendre (Chebyshev) collocation method based on a Birkhoff interpolation [6, 17] such that the corresponding system of linear equations is well-conditioned and the condition numbers do not depend on N, and their approach produces the exact inverse of the pseudospectral differentiation matrix of the highest derivative with only interior collocation points involved. The minimal eigenvalue of the second Jacobi pseudospectral differentiation matrix is a constant, so the differential operator of the highest order and the underlying boundary conditions can be associated with a suitable Birkhoff interpolation.

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This opens the way to a new well-conditioned Jacobi-collocation method with another basis, to produce optimal integration preconditioners for usual collocation methods for exact boundary conditions. We provide such a new collocation scheme, where simulations for second order differential equations for example show both stability and high accuracy. However, numerical simulations in various areas of application (e.g. in quantum mechanics, biology, or financial mathematics) involve differential equations on unbounded domains, so the second part of this article is devoted to alternative Laguerre and Hermite collocation methods. Further, if the smallest eigenvalues of the corresponding matrices depend on their dimensions [24] such that these methods cannot be used, we construct new Birkhoff interpolation basis functions to produce both well-conditioned systems of linear algebraic equations and optimal preconditioners. The corresponding collocation schemes for second order differential equations with Dirichlet boundary conditions demonstrate high accuracy and improved stability. In Section 2, the interpolation basis uses Jacobi-Gauss-Lobatto (JGL) points. In Section 3 and Section 4, Laguerre-Gauss-Radau (LGR) and Hermite-Gauss points are adopted for the construction of new bases. All of these bases are incorporated in the corresponding collocation schemes used in the numerical simulations. Our concluding remarks are in Section 5.

2. Motivations and Observations from Collocation on a Finite Interval

In this section, we extend the well-conditioned collocation method from Ref. [23] to general Jacobi-Gauss-type points. Our goal is to develop new collocation schemes for unbounded domains.

2.1. Birkhoff interpolation basis on Jacobi-Gauss-Lobatto (JGL) points

Let $\{h_j\}$ be the Lagrange interpolating polynomials associated with the JGL points $\{x_j\}_{j=0}^{N}$ where $x_0=-x_N=-1$ [19]. The differentiation matrices are defined as

$$\boldsymbol{D}^{(k)}=\big(d_{ij}^{(k)}\big)_{0\le i,j\le N}\,,\quad \boldsymbol{D}_{\rm in}^{(k)}=\big(d_{ij}^{(k)}\big)_{1\le i,j\le N-1}\,,\quad d_{ij}^{(k)}=h_j^{(k)}(x_i)\,,$$

and we set $\boldsymbol{D}:=\boldsymbol{D}^{(1)}$ and $\boldsymbol{D}_{\rm in}:=\boldsymbol{D}_{\rm in}^{(1)}$. Explicit formulas for the entries of the matrix $\boldsymbol{D}$ and the relation are [19]

$$\boldsymbol{D}^{(k)}=\boldsymbol{D}\boldsymbol{D}\cdots\boldsymbol{D}=\boldsymbol{D}^k,\quad k\ge 1\,.$$

It is also known that the condition numbers of the matrices $\boldsymbol{D}_{\rm in}^{(k)}$ grow like N^{2k} — cf. Refs. [2,25]. We are particularly interested in the second-order differentiation matrix. Weideman & Trefethen [25] studied eigenvalues of the pseudospectral second derivative matrix with homogeneous Dirichlet boundary conditions, and observed that only about $2N/\pi$ of the eigenvalues of the continuous operator are accurately approximated by the eigenvalues of the discrete operator. Vandeven [22] proposed a rigorous proof of that conjecture for the Galerkin Legendre spectral method, and Welfert [26] showed his results are also valid for the Legendre pseudospectral collocation method. Analogously, in the general Jacobi case the smallest eigenvalue of the matrix $-\boldsymbol{D}_{\rm in}^{(2)}$ can be approximated by $\pi^2/4\approx 2.467$.