

# Well-Conditioned Spectral Collocation Methods for Problems in Unbounded Domains

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Received 23 June 2019; Accepted (in revised version) 13 September 2019

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**Abstract.** Based on the generalized Laguerre and Hermite functions, we construct two types of Birkhoff-type interpolation basis functions. The explicit expressions are derived, and fast and stable algorithms are provided for computing these basis functions. As applications, some well-conditioned collocation methods are proposed for solving various second-order differential equations in unbounded domains. Numerical experiments illustrate that our collocation methods are more efficient than the standard Laguerre/Hermite collocation approaches.

**AMS subject classifications:** 65N35, 65M70, 33C45, 41A05, 41A30

**Key words:** Spectral collocation methods, generalized Laguerre and Hermite functions, Birkhoff interpolation, fast and stable algorithms.

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## 1. Introduction

Many practical problems arising in science and engineering are set in unbounded domains, and some significant progress has been made in using spectral methods for solving such kinds of problems. Among the existing work, the Laguerre and Hermite spectral methods are the most popular ones and have been widely used over the past few decades, see, e.g., [11, 13, 14, 16, 17, 23, 26, 27, 32, 34, 35].

For differential equations on the half line, one usually considered approximations by the standard Laguerre polynomials with the weight function  $e^{-x}$ . However, the standard Laguerre spectral method is not appropriate for problems with variable coefficients. For example, if we study the numerical solutions of the Black-Scholes equations in financial mathematics, it is natural to use the generalized Laguerre approximation

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with the weight function  $x^2 e^{-x}$ . Moreover, if we consider the spherically symmetric problems arising in quantum mechanics, we also have to use the generalized Laguerre functions. Furthermore, the asymptotic behaviors of exact solutions at infinity usually depend on some parameters in the underlying differential equations. Thus, it seems reasonable to adopt the generalized Laguerre orthogonal systems with a more general weight function  $\omega_{\alpha,\beta}(x) = x^\alpha e^{-\beta x}$ . In fact, by proper selection of parameter  $\beta$ , the numerical solutions could fit the asymptotic behaviors of exact solutions at infinity more properly. For differential equations on the whole line, it is also more appropriate to use generalized Hermite functions with some scaled parameter for numerical simulations. As pointed out in [25], the standard Hermite functions sometimes work poorly in practice, and too many Hermite functions are required to approximate differential equations.

Among several versions of spectral algorithms, the spectral collocation method is implemented straightforwardly in physical space, and performs differentiations on a set of preassigned collocation points, where the equation under consideration is satisfied, so it has remarkable advantages in dealing with variable coefficients or nonlinear problems. However, the researchers are oftentimes plagued by severe ill-conditioning of the differentiation matrix. It is well-known that the construction of suitable preconditioners is an effective approach to circumvent this barrier. Many considerable contributions have been made in preconditioning spectral methods on finite domains. The successful attempts particularly include preconditioning usual collocation schemes by low-order finite difference or finite elements [1, 2, 7, 8, 20, 21], and preconditioning differentiation by integration [3, 5, 6, 9, 10, 12, 19, 28, 30, 36]. Recently, Costabile and Longo [4] proposed the Birkhoff-Lagrange collocation methods for boundary value problems using some interpolating basis polynomials associated with suitable Birkhoff interpolation problems (cf. also [22]). Wang et al. [28] showed that such an approach led to well-conditioned collocation schemes and offered optimal preconditioners for usual collocation schemes in bounded domains. Some follow-ups and extensions of the Birkhoff collocation notions can also be found in [29, 38]. For problems defined in unbounded domains, Zhang et al. [39] proposed the Birkhoff collocation methods based on the standard Laguerre and Hermite functions.

The purpose of this paper is to extend the work of [39] to more general situations, such that the basis functions can match asymptotic behaviors of exact solutions at infinity more appropriately. To this end, we construct two sets of Birkhoff basis functions based on the generalized Laguerre and Hermite functions in unbounded domains. The new basis functions can be explicitly achieved. We also provide fast and stable approaches to compute these basis functions. Furthermore, we propose spectral collocation methods based on the Birkhoff basis functions for second-order problems in unbounded domains. Numerical results are provided to show the advantages of the suggested methods.

The rest of the paper is organized as follows. In Section 2, we first introduce the generalized Laguerre functions and their important properties. Then we construct the Laguerre-Birkhoff basis functions and provide an efficient algorithm. We also present