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Using Gaussian Eigenfunctions to Solve Boundary Value Problems

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This is dedicated to Graeme Fairweather, whose guidance and patience has instilled an everlasting love of mathematics in myself and countless others.

Abstract. Kernel-based methods are popular in computer graphics, machine learning, and statistics, among other fields; because they do not require meshing of the domain under consideration, higher dimensions and complicated domains can be managed with reasonable effort. Traditionally, the high order of accuracy associated with these methods has been tempered by ill-conditioning, which arises when highly smooth kernels are used to conduct the approximation. Recent advances in representing Gaussians using eigenfunctions have proven successful at avoiding this destabilization in scattered data approximation problems. This paper will extend these techniques to the solution of boundary value problems using collocation. The method of particular solutions will also be considered for elliptic problems, using Gaussian eigenfunctions to stably produce an approximate particular solution.

AMS subject classifications: 65N35, 65N80

Key words: Meshless method, method of particular solutions, boundary value problem.

1 Introduction

Kernel-based meshfree approximation methods have gained popularity in several fields, including scattered data interpolation [52], finance [25], statistics [49], machine learning [43] and others. One of the great benefits of using these methods is that no discretization of the relevant domain is required; basis functions are centered at various points throughout the domain, allowing for kernel-based methods to circumvent some of the barriers associated with higher dimensional problems. Additionally, a variety of kernels

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exist, providing users in each application the ability to tailor the solution basis to fit that application's specific opportunities and constraints.

Techniques for solving boundary value problems (BVPs) with radial basis functions (RBFs) have advanced significantly in the past two decades. The original method for solving elliptic partial differential equations (PDEs) with RBFs came in 1990 [31] and involved an unsymmetric collocation of basis functions at points chosen throughout the domain. Since that initial work, further analysis has been done on the convergence of this collocation method [46], which has encouraged its use despite its theoretic potential for failure [26]. A symmetric collocation technique was also developed [9] which ensured invertibility of the collocation system by using a modified set of basis functions.

Another popular method for solving BVP with radial basis functions is the method of fundamental solutions [8]. Essentially, this method replaces the BVP with an interpolation problem on the boundary using functions which satisfy the PDE. The mathematical formulation of this method is well-developed, but it is only applicable for homogeneous problems where the fundamental solution is known. The method of particular solutions [5] is an adaptation for inhomogeneous problems involving two approximation systems: one to satisfy the inhomogeneity in the interior, and another to satisfy the boundary conditions, assuming a now homogeneous problem. The use of radial basis functions to approximate particular solutions was discussed in [21, 27].

One of the great shortcomings of radial basis functions is that, for some parameterizations, the resulting linear system may be irrevocably ill-conditioned [10]. Even more troublesome is the fact that the most accurate parameterizations may lie in the ill-conditioned regime [19]. This ill-conditioning is especially significant for kernels with a great deal of smoothness, which often tempers the optimism of researchers hoping to exploit their spectral accuracy. In [11], this problem was addressed for Gaussians in $\mathbb{R}^d$ by using a truncated eigenfunction expansion of the Gaussian. Here, we will extend the approximation via eigenfunctions to the solution of boundary value problems.

Many more methods for solving boundary value problems with kernels exist beyond what will be discussed in this paper. Multilevel methods [30, 36] have been presented, including for higher order problems [1], to attempt to mitigate the cost associated with solving dense systems generated by globally supported RBFs. Finite difference schemes based on RBFs [13, 14] have proven to be an effective meshfree solver for geological and climate based problems. Partition of unity methods [34] are being developed now to incorporate RBF collocation with other solution schemes for applications including crack propagation. Petrov-Galerkin techniques [2] have been developed to allow the weak form solution of PDEs, while recent work [47] has provided analytic support for this approach. Some work has been done incorporating RBFs into discontinuous Galerkin schemes [44]. Kernel based PDE solvers on manifolds [20] are beginning to mature as well.

To narrow our focus from all possible BVP solvers using kernels, we will discuss only collocation and the method of particular solutions. In Section 2 we consider the solution of boundary value problems by collocation with traditional Gaussian RBFs, and demon-