Generating efficient basis sets for unbounded domains

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Abstract. The treatment of the problems involving unbounded domains (UDs) with vanishing boundary conditions is always challenging. For spectral methods, in particular, very limited basis sets are commonly used for such domains, in which the ranges of the decay rates with acceptable computational efficiency, are very small. Furthermore, maintaining high level of analyticity becomes burdensome. Developing efficient mapped basis tailored for such problem is one of the main strategies to overcome these difficulties. In this work, we present a technique to generate efficient basis sets for UDs. This approach allows using basis sets defined for bounded domains (BDs) for problems in UDs, and hence, providing more freedom to choose from a variety of basis sets. To ensure computational efficiency, the designed transformations cover a wide range of decay rates and allow solving integrals analytically. The method is applied to solve many differential equations encountered frequently in many physics related problems. The results illustrate the efficiency of the developed technique and mapped basis sets.

1. Introduction

Many physical problems involve unbounded domains (UDs) with vanishing boundary conditions. Solving such problems is challenging. In spectral methods, various basis sets are commonly used for such domain such as Hermite and sinc function. However, the ranges of decay rates in which these basis sets are efficient are very small, and hence cannot be used in approximation of functions with wide range of decay rates \([1, 2, 3, 4]\). The other possibility is to transform the UD to a BD. The advantage of transformation is that we can exploit the basis sets which only applicable to the BDs. Hence, there is more freedom and flexibility in the choice of basis sets. The simplest way to convert an UD to a BD is by chopping the domain. Such method introduces a truncation error, and hence it is not a good option where higher accuracies are required. Of course the truncation error can be reduced by increasing the domain size, but at an increased computational cost. Another possibility is to convert UD to a BD through domain mapping. The main advantage of domain mapping is that there is no truncation error and a variety of basis sets which are only applicable to BDs can now be implemented for the problems involving UDs.

The idea of domain transformation may seem simple, and although there are unlimited ways to transform an UD to a BD \([1]\), however, transforming the domain, and at the same time...
not making the problem complex (i.e keeping integrals simple and analytically solvable) and approximating a wide range of decay rates is challenging.

In this work, we present an efficient approach to map a UD to a BD using using generalized coordinate transformation [5]. After the transformation, any basis set defined for any BD can be implemented to solve the problem. The developed method ensures orthogonality and a major portion of the problems can be solved analytically. This increases the computational efficiency and accuracy. Most importantly, the approach approximates efficiently various type of decaying functions with a wide range of decay rates by appropriate choices of mapping and basis functions. The choice of basis functions also affect the resulting integrals. Hence, using simple basis sets helps in simplifying the integrals involved, and hence increasing computational efficiency.

The basis set used in this paper is Fourier sine series \( \sin(k\pi x) \), which is an orthogonal basis set in the domain \((0,1)\). Hence, the UD is mapped to BD \((0,1)\). The mapping is tested on a first order differential equation. It is shown that a wide range of decays that can be approximated efficiently and accurately.

2. Formulation

A transformation function can be defined as:

\[
 x = h(u), \quad u = h^{-1}(x) = g(x), \quad x \in (-\infty, \infty), u \in (a,b)
\]

(1)

There are infinite possibilities for such transformations [5, 6, 1, 2]. For any orthogonal basis set \( \{P_k(u)\} \) defined in a BD, we seek an orthogonal basis set defined in UD of the form

\[
 f_k(x) = P_k(g(x))\mu_r(g(x)),
\]

(2)

where \( \mu_r(g(x)) \) is an auxiliary function to ensure the vanishing boundary conditions are satisfied. Since we assume \( f_k(x) \) is orthogonal, the following relationship must be satisfied:

\[
 \int_{-\infty}^{\infty} f_k(x)f_l(x)dx = \delta_{kl}
\]

(3)

Coordinate transformation, will result in the following form

\[
 \int_{a}^{b} P_k(u)P_l(u)\mu_r^2(u)\frac{dx}{du}du = \delta_{kl}
\]

(4)

Since \( \{P_k(u)\} \) is orthogonal in the domain \((a, b)\) with respect to weight function \( w(u) \), we can write

\[
 \int_{a}^{b} P_k(u)P_l(u)w(u)du = c_k\delta_{kl}.
\]

(5)

Comparing equations (4) and (5), we get:

\[
 \frac{dx}{du} = \frac{w(u)}{c_k\mu_r^2(u)}
\]

(6)

which shows that \( \mu(u) \) plays a key role in the transformations. Solving equation 6 for a unique \( \mu_r(u) \) will result in a unique transformation function, which can be used to map the problem from UD to BD.
Table 1. Transformations functions $x = h(u)$ [1].

| Symbol | $\mu_r(u)$ | $x(u)$ |
|--------|------------|--------|
| $T_1$  | $\sin\frac{1}{2}(\pi u)$ | $\frac{2}{\pi} \log\left[\tan\left(\frac{\pi u}{2}\right)\right]$ |
| $T_2$  | $\sin(\pi u)$ | $-\frac{2}{\pi} \cot(\pi u)$ |

3. Implementation

The proposed method can be implemented to approximate/solve any function/ODE/PDEs defined in the UDs, provided that the vanishing boundary conditions are satisfied. Here, we present a generalized case of a forced function ODE problem given by:

$$\hat{L}\psi(x) = F(x),$$

and its approximate function/solution can be written in the form of summation of basis set $f_l(x)$ as:

$$\psi(x) \approx \sum_{l=1}^{N} a_l f_l(x)$$

The matrix form of equation 7 can be written as:

$$L a = \Gamma$$

where $L$ and $\Gamma$ are given by:

$$[L]_{kl} = \int_{a}^{b} f_k(u) \hat{L}(f_l(u)) \frac{w(u)}{c_k \mu_r^2(u)} du$$

$$[\Gamma]_{k} = \int_{a}^{b} f_k(u) F(h(u)) \frac{w(u)}{c_k \mu_r^2(u)} du$$

By proper choice of basis set, $L$ can be calculated analytically, and then $a$ can be computed, which gives the final solution.

4. Results and Discussions

To test the proposed method, we have chosen our complete basis set to be sine functions. However, any other proper basis set can be used. The complete basis set is given by equation 2, where

$$P_k(g(x)) = P_k(u) = \sin(k\pi u)$$

and

$$\mu_r(g(x)) = \mu_r(u) = \sin^{r}(\pi u), \quad r \in N_1$$

The transformation functions resulting from the chosen auxiliary function are given in Table 1.

The developed method is validated with two case studies. The 1st case study (Case I) involves the implementation of the developed method to a simple 1st order differential equation i.e. $\hat{L} = \frac{d}{dx}$, while the 2nd case study (Case II) involves a more generic 2nd order differential equation with constant coefficients i.e. $\hat{L} = L_2 \frac{d^2}{dx^2} + L_1 \frac{d}{dx} + L_0$. In both case studies, the obtained
results are compared with the results obtained using Hermite basis to show the accuracy and efficiency of the developed method. Furthermore, for comparison purposes, the exact solution (for both case studies) is assumed to be known and is given by:

$$\psi(x) = \cos(\kappa x)e^{-\alpha x^2}$$  \hspace{1cm} (14)

where $\kappa = 2$ and $\alpha \in (10^{-2} - 10^4)$.

The results of Case I are plotted in Figure 1 where we have computed the required number of basis functions to achieve an accuracy of $10^{-10}$ at different decay rates ($\alpha$). As can be seen from the results, Hermite is more accurate for lower decay rates whereas the developed method is more accurate for higher decay rates. However, this can be changed through proper scaling. The point of significant importance is the range of decay rates in which a method is efficient, and this is evident from the Figure 1 that the developed method covers a wider range of decay rates and hence can be implemented to physical problems which involves wide range of decaying functions.

![Figure 1. $N$ needed to achieve $\varepsilon < 10^{-10}$ for various values of $\alpha$.](image)

The Case II is presented to better quantify the range of decay rates that can be covered efficiently using the proposed method. For this case, we have considered a 2nd order differential equation with constant coefficients given by:

$$L_2 \frac{d^2}{dx^2} + L_1 \frac{d}{dx} + L_0 = F(x)$$  \hspace{1cm} (15)

where $L_2 = L_1 = L_0 = 1$. Case II provides a quantitative measure of how much wider range of decay rates can be covered by a particular method. The quantitative measure used is the order of magnitude (OM). The OM is computed for $N = (100, 200$ and $300)$, and the results are given in Figure 2. As can be seen from the results, both transformation functions ($T_1$ and $T_2$) outperform Hermite for any number of basis functions. An OM of greater than 3.5 can be achieved using the transformation function $T_2$. All the results indicate that the developed method is very efficient, accurate and covers a much wider range of decay rates compare to Hermite. This opens a new world of possibilities of basis sets for the unbounded domains.

5. Conclusion

Problems involving unbounded domains with vanishing boundary conditions are challenging because of the limited basis sets available for these domains. On the contrary, there is an abundance of basis sets for the problems in bounded domains. Therefore, we have proposed a generalized method of coordinate transformation to convert an unbounded domain to a bounded
one without losing any information (truncation error). Furthermore, the proposed method also takes into consideration the orthogonality, the need to cover a wide range of decay rates, and solving integrals analytically. Hence, properly designed transformations can potentially unlock the doors to a new world of basis functions for unbounded domains.

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Figure 2. $N$ needed to achieve $\varepsilon < 10^{-10}$ for various values of $\alpha$. 