Deformation and Smoothing of Cusp Singularities

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Abstract. A cusp singularity (CS), is a point at which the slope of a continuous curve changes abruptly in sign and magnitude. A particular type of CS, which is the focus of this paper, is where only the sign of the slope is altered while the magnitude of the slope is unchanged. This type of CSs occur in many natural phenomena such as Kato’s cusp and particular plasmonics. Solving such problems numerically can be challenging because of the discontinuity in the derivatives. In this paper, we present an efficient spectral method incorporated with transformation (mapping) to handle the cusp problem. The transformation is based on functions that are locally odd around all the cusp points. The idea is to transform functions from $C^0$ continuity to $C^N$ continuity ($N > 1$), and then implement a spectral method to solve the mapped problem without any domain decomposition. The final solution is obtained with inverse mapping.

1. Introduction

A cusp is a point at which a continuous function possesses a discontinuity in its first derivative [1]. A particular case of cusp, which is the focus of this paper, is where the magnitude of the slope on both sides of the cusp is equal but opposite in sign. Such type of cusps appear naturally in many physical problems such as Kato’s cusp condition in the atomic structure calculations. Other real life examples of cusps include caustics, wave fronts and some particular plasmonics.

Different numerical techniques are used to solve the cusp problem numerically. Most of the approaches involve domain discretization including different mesh-based and multi-domain mesh-free methods [2, 3, 4, 5, 6, 7, 8, 9, 10]. In domain discretization the computational domain is divided into sub-domains (multi-domain mesh-free methods) or in the form or a grid (mesh-based methods) such that the cusps appear at the boundaries of the domain (or at the grid points). In either case, cusp boundary conditions can be easily enforced. However, domain discretization can become costly for bigger systems with multiple cusp points. For $M$ cusp points, the required sub-domains or grid size is $M + 1$, and the computational cost will increase by $(M + 1)^n$ for an n-dimensional problem.

This paper focuses on solving the problems involving special cusp singularities using spectral method without any domain discretization. Hence higher accuracies can be achieved at a relatively lower computational cost. However, the spectral methods cannot be implemented directly to such problems because of the Gibb’s phenomenon which occurs naturally in approximating discontinuous functions using continuous differentiable functions [11]. To tackle this issue, this paper proposes transformation (mapping), to completely eliminate all the cusp...
singularities. The idea is to transform the $C^0$ continuous function to $C^N$ continuous function where $N>1$ using an auxiliary function that is locally odd around the cusp points. The resulting smooth $C^N$ continuous function is $N$ times differentiable, and hence can be approximated with higher accuracy and efficiency using a high-order method. Care needs to be taken in the choice of the auxiliary function to ensure that the proposed method can be implemented to the problems in higher dimensions as well without making the method more complicated. To achieve this, the auxiliary function is chosen to be a separable function so that tensoral construction can be used for higher dimensions from 1-D formulation. Using tensor product significantly reduced the computational cost and increases the efficiency of the method. Furthermore, higher continuity (i.e. higher “$N$”) will result in higher accuracy and the continuity should not be less than the order of the differential equation i.e. for a second order differential equation, the mapped function should be at least $C^2$ continuous. The mapped function can then be approximated with very higher actuaries at relatively lower computational cost using any high-order method.

The formulation is presented in this paper is generalized, so, any proper spectral method incorporated with transformation can be used to approximate functions and solve differential equations containing multiple cusp singularities. For the purpose of presenting some results, we have chosen sine series as our basis set for the high-order method. So our computational domain is between 0 and 1 (sine series is orthonormal between 0 and 1 with boundary conditions $f(0) = 0$ and $f(1) = 0$). Different cusp points (arbitrary chosen) are used for validation. To assess the accuracy of the method, a relative error ($E_{rel}$) is computed by comparing the approximate solution with the exact solution. A very good agreement between the exact and approximate solutions is achieved using only 100 basis functions resulting in accuracies better than $10^{-11}$.

2. Transformation of Function from $C^0$ to $C^N$ Continuity

Because of the symmetrical nature of the considered cusp family, it is possible to transform the problem from $C^0$ continuity to $C^N$ continuity ($N>1$) using some auxiliary function. Let $\psi(x)$ be a function containing $M$ cusps at points $\{x_1, x_2 \cdots x_M\}$ (CS). We assume that there exists an auxiliary function $\eta(x)$ such that

$$\tilde{\psi}(x) = \psi(x)\eta(x)$$

where $\tilde{\psi}(x)$ is $C^N$ continuous with $N>1$, and $\eta(x)$ is given by

$$\eta(x) = \prod_{p=1}^{M} \zeta(x - x_p)$$

where $M$ is the total number of cusp points, $x_p$ is the location of $p^{th}$ cusp and $\zeta(x)$ is a function which is locally odd (around the cusp point). With proper choice of $\zeta(x)$, the resulting mapped function $\tilde{\psi}(x)$ becomes $C^N$ continuous. After the transformation, we seek spectral numerical solution for the function $\tilde{\psi}(x)$ which is $C^N$ continuous. The spectral method is implemented to the whole domain without any discretization. The actual function $\psi(x)$ can be obtained by inverse mapping.

It is very crucial to ensure that the $\eta(x)$ should result in $\tilde{\psi}(x)$ which is continuously differentiable. This is because the order of continuity of $\tilde{\psi}(x)$ will define the order of differential equation that can be solved efficiently using the proposed technique. If the chosen $\eta(x)$ results in the mapped function $\tilde{\psi}(x)$ which is $N$ times differentiable, then the auxiliary function can be used to solve any $N^{th}$ order differential equation. This is depicted in Figure 1, where $\zeta = x$ (which is an odd function) is chosen as the auxiliary function. As can be seen from Figure 1, $\zeta = x$ result in the mapped function which is $C^1$ continuous, and hence it can only be used in approximation or solving $1^{st}$ order differential equations. On the other hand, $\zeta = x^3$ results in the mapped function which is $C^2$ continuous, and hence can be used for approximation as well.
as 2nd order differential equations (Figure 2). Hence, the choice of auxiliary function is the key to unlock the full potential of this method.

The proposed idea can be extended to higher dimensions using tensoral construction provided that the chosen basis set and the auxiliary function are separable. Hence, for an n-dimensional (nD) function \( \psi(\mathbf{r}) \) containing multiple cusps, we assume there exists an nD auxiliary function \( \eta(\mathbf{r}) \) such that

\[
\tilde{\psi}(\mathbf{r}) = \psi(\mathbf{r})\eta(\mathbf{r})
\]

where \( \tilde{\psi}(\mathbf{r}) \) is C\( N \) continuous with \( N > 1 \), and \( \eta(\mathbf{r}) \) is separable. For an nD problem with \( M \) cusp points, the auxiliary function \( \eta(\mathbf{r}) \) is given by

\[
\eta(\mathbf{r}) = \prod_{d=1}^{n} \eta_d(x_d) = \prod_{d=1}^{n} \prod_{p=1}^{M} \zeta_d(x_d - x_{d,p})
\]

where \( x_d \) is the \( d^{th} \) coordinate variable and \( x_{d,p} \) is the position of the \( p^{th} \) cusp point corresponding to the \( d^{th} \) coordinate variable. After the transformation, any proper spectral method can be implemented to solve the modified problem [12, 13, 14], and the actual results can be obtained by inverse mapping.
3. Implementations and Formulations
In this section, the formulation for implementing the proposed method within the frame of spectral methods is presented. At the beginning, we start with approximation problem and follow that with the implementation to 2nd ordinary differential equation. This is followed by an extension to nD problems utilizing tensoral construction.

3.1. Implementation to Approximation of Functions Containing Multiple CS
3.1.1. Implementation to 1D problems
Let the function to be approximated is given by
\[
\psi(x) = F(x), \quad x \in (a, b)
\] (5)
where \(\psi(x)\) has multiple CS and all the CS are defined within the domain \((a, b)\). After applying transformation using Eq. (1), we get
\[
\tilde{\psi}(x) = F(x), \quad \eta(x) = F(x)
\] (6)
Clearly the left side of the equation will have multiple pole (at the cusp points) because the auxiliary function \(\eta(x)\) is zero at these points. Therefore, we must rearrange Eq. (6) in order to avoid the singularities that may result in divergence of the integrals. Hence, we rearrange Eq. (6) as
\[
\tilde{\psi}(x) = \gamma(x)
\] (7)
where
\[
\gamma(x) = F(x)\eta(x)
\] (8)
Now we can implement any spectral method to solve Eq. (7). The approximate solution is written in the form of summation of the basis function as
\[
\tilde{\psi}(x) \approx \sum_{l=1}^{M} a_l f_l(x)
\] (9)
where \(f_l(x)\) represent a basis function. We apply the approximate solution to Eq. (7), and take the inner product with respect to \(f_k(x)\) to obtain the matrix form of Eq. (7) which is given by
\[
D_0 a = \Gamma
\] (10)
where \(a\) is the vector containing all the expansion coefficients, and the matrix \(D_0\) is computed as
\[
[D_0]_{kl} = \int_{a}^{b} f_k(x)f_l(x)dx
\] (11)
and the vector \(\Gamma\) is calculated as
\[
[\Gamma]_k = \int_{a}^{b} f_k(x)\gamma(x)dx
\] (12)
Once the coefficients are calculated, the approximate solution can be found using Eq. (9). Finally, the original solution can be obtained using inverse transformation (using Eq. (1)).
3.1.2. Extension to n-D problems

The extension to the higher dimension using tensoral construction depend solely on the choice of the basis set and the auxiliary function. If the chosen basis set and the auxiliary functions are separable, then the property of tensoral construction can be exploited to build any higher dimension matrices from the corresponding 1-D matrices.

Let the function to be approximated is given by \( \psi(r) \), which is an n-D function with \( M \) cusp points located at \( \{r_1, r_2, \cdots, r_M\} \). \( \psi(r) \) can by written as:

\[
\psi(r) = F(r), \quad r \in (a, b)
\]  

Using the formulation proposed in Section 2, we can modify Eq. (13) as:

\[
\tilde{\psi}(r) = \gamma(r)
\]

where

\[
\gamma(r) = F(r)\eta(r)
\]

where \( \eta(r) \) is a separable function, and since the chosen basis set is also separable, the approximate solution can be written as:

\[
\tilde{\psi}(r) = \sum_{l_1} \sum_{l_2} \cdots \sum_{l_n} a_{l_1 l_2 \cdots l_n} f_L(r), \quad \text{where} \quad f_L(r) = f_{l_1}(x_1)f_{l_2}(x_2)\cdots f_{l_n}(x_n)
\]

The matrix form of Eq. (14) is given by

\[
D_{0,nD} a_{nD} = \Gamma_{nD}
\]

where \( D_{0,nD} \) can be obtained from the corresponding 1-D matrices as follows:

\[
D_{0,nD} = \bigotimes_{i=1}^{j} D_{0,x_i} \bigotimes_{j=1}^{n} D_{0,x_n}
\]

where \( \otimes \) is the Kronecker product operator and \( D_{0,x_j} \) is the \( j^{th} \) 1-D matrix calculated using Eq. (11). The vector \( \Gamma_{nD} \) is calculated as

\[
\Gamma_{nD} = \int_a^b \cdots \int_a^b f_k(r)\gamma(r)dr
\]

After calculating the approximate solution, the final solution is obtained using inverse mapping.

3.2. Implementation to Differential Equations

3.2.1. Implementation of ODEs

In this work, we limit ourselves to 2\textsuperscript{nd} order differential equations though the method can be implemented to higher order differential equation. Here, we consider 2\textsuperscript{nd} order ODE with constant coefficients involving the source function \( F(x) \) can be written as:

\[
L_2 \frac{d^2}{dx^2} \psi(x) + L_1 \frac{d}{dx} \psi(x) + L_0 \psi(x) = F(x)
\]

where \( L_2, L_1 \) and \( L_0 \) are constants, and \( \psi(x) \) is a \( C^0 \) function containing multiple CS. Using the same idea from the previous sections, we transform \( \psi(x) \) to \( \tilde{\psi}(x) \) using Eq. (1). Also, we need to ensure that the singularities are completely removed from the equation. To achieve that, we modify Eq. (20) as:

\[
\eta(x) \left[ L_2 \frac{d^2}{dx^2} \left( \frac{\tilde{\psi}(x)}{\eta(x)} \right) + L_1 \frac{d}{dx} \left( \frac{\tilde{\psi}(x)}{\eta(x)} \right) + L_0 \left( \frac{\tilde{\psi}(x)}{\eta(x)} \right) \right] = \gamma(x)
\]
where $\gamma(x)$ is given by Eq. (8). To solve Eq. (21), using high-order method, the assumed approximate solution is given by Eq. (9). The matrix form of Eq. (21), which is given by

$$(L_2D_2 + L_1D_1 + L_0D_0)\mathbf{a} = \Gamma$$

(22)

where $D_0$, and $\Gamma$ are calculated using Eq. (11) and Eq. (12), respectively, whereas the matrices $D_2$, $D_1$ and are computed as:

$$[D_2]_{kl} = \int_a^b f_k(x) \left(f_1''(x) - 2f_1'(x)\sigma(x) - f_1(x)\sigma'(x) + f_1(x)\sigma(x)^2\right) dx$$

(23)

and

$$[D_1]_{kl} = \int_a^b f_k(x) \left(f_1'(x) - f_1(x)\sigma(x)\right) dx$$

(24)

where $f_1'(x)$ and $f_1''(x)$ are first and second derivatives of $f_1(x)$, respectively, and $\sigma'(x)$ is the first derivative of $\sigma(x)$ which is given by

$$\sigma(x) = \sum_{i=1}^{N} \frac{d}{dx}\frac{\zeta(x-x_i)}{\zeta(x-x_i)}$$

(25)

and

$$\sigma'(x) = \sum_{i=1}^{N} \left[ \frac{d^2}{dx^2}\frac{\zeta(x-x_i)}{\zeta(x-x_i)} - \left(\frac{d}{dx}\frac{\zeta(x-x_i)}{\zeta(x-x_i)}\right)^2 \right].$$

(26)

Once $D_2$, $D_1$, $D_0$ and $\Gamma$ are computed, the unknown coefficients can be calculated by algebraically solving Eq. (22).

### 3.3. Extension to PDEs

A general n-dimensional PDE is given by

$$\hat{L}\psi(r) = F(r)$$

(27)

where $\hat{L}$ can be any differential operator, and $r$ is a spatial vector. For an n-D problem, $r = \{x_1, x_2, \ldots, x_n\}$, $\psi(r)$ is $C^0$ continuous function, and has $M$ cusps at points $\{r_1, r_2, \ldots, r_M\}$. Using the transformation proposed in Section 2, the n-D PDE given in Eq. (27) can be modified as:

$$\hat{L}\left[\frac{\tilde{\psi}(r)}{\eta(r)}\right] = F(r)$$

(28)

Again, we limit ourselves to 2nd order differential equation. Hence, the operator $\hat{L}$ is composed of first and second derivatives only. This operator can be written in compact form as:

$$\hat{L} = \sum_{i=1}^{n} \sum_{j=i}^{n} v_{ij}(r) \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{n} w_i(r) \frac{\partial}{\partial x_i} + \kappa$$

(29)

where $v_{ij}(r)$ and $w_i(r)$ are scalar functions. If we apply the above operator to Eq. (28), we need to ensure that all the singularities are removed. This is achieved by multiplying the operator $\hat{L}$ by $\eta(r)$. The modified equation is given by

$$\eta(r) \left[\sum_{i=1}^{n} \sum_{j=i}^{n} v_{ij}(r) \frac{\partial^2}{\partial x_i \partial x_j} \left(\frac{\tilde{\psi}(r)}{\eta(r)}\right) + \sum_{i=1}^{n} w_i(r) \frac{\partial}{\partial x_i} \left(\frac{\tilde{\psi}(r)}{\eta(r)}\right) + \kappa \left(\frac{\tilde{\psi}(r)}{\eta(r)}\right)\right] = \gamma(r)$$

(30)
As aforementioned, both the basis set and the auxiliary functions are separable, hence, we can exploit the same idea that we used in the approximation of n-D functions, which is tensoral construction of higher dimensional matrices using the corresponding 1-D matrices. Using the approximate solution given by Eq. (16), the matrix form of Eq. (30) is given by

\[
[D_{2,nD} + D_{1,nD} + D_{0,nD}] \mathbf{a}_{nD} = \mathbf{\Gamma}_{nD}
\]  

(31)

The matrices \(D_{2,nD}, D_{1,nD}\) and \(D_{0,nD}\) can be calculated using the corresponding 1-D matrices in a similar fashion which is used Subsection 3.1.2 (Eq. 18). After computing the matrices, the unknown coefficients are calculated which are then used to calculated the approximate mapped solution. The final solution is obtained by inverse mapping.

4. Results and Discussions

To demonstrate the accuracy and efficiency of the method, we have presented a case study in which the developed scheme is implemented to approximate a function with multiple cusp singularities. As mentioned previously, any proper spectral method can be implemented using the proposed approach. In this work, the chosen basis set is sine series i.e. \(f_l(x) = \sin(l \pi x)\), which is an orthonormal basis set for the domain (0,1) with boundary conditions \(\psi(0) = 0\) and \(\psi(1) = 0\). The function to be approximated is given by

\[
\psi(x) = \prod_{p=1}^{M} \sqrt{(x - x_p)^2 \sin^2(x)} , \quad x \in (0,1)
\]

(32)

where \(M\) is the total number of cusp points and \(x_p\) is the location of \(p^{th}\) cusp point. The chosen auxiliary function is given by:

\[
\zeta(x) = \sin^2(x - x_p)
\]

(33)

For this work, we only focus on the approximation of functions in 1D, however, idea is extendable to higher dimensions as well as differential equations. The function to be approximated is given by Eq. (32). Three cusp points (chosen randomly) are considered. The cusp points are located at \(x_p = \{0.40, 0.53, 0.68\}\), and the results are shown in Figures 3 and 4. Results show a very good agreement between the exact and the approximate function. A relative error (\(E_R\)) exceeding \(10^{-11}\) is achieved using only 100 basis functions.

![Figure 3. A comparison of the exact and the approximate functions in 1-D (multiple cusp points).](image1)

![Figure 4. A comparison of \(E_R\) computed with and without mapping for the approximation of functions in 1-D.](image2)
5. Conclusion
The cusp problem is challenging because of the discontinuity in the first derivative. The well-developed high order methods are very efficient and accurate in approximating continuous differentiable functions. However, they are not efficient for C⁰ continuous functions. In this paper, we have proposed a simple approach which is based on transformation of the C⁰ continuous function to Cᴺ continuous function (N>1) using an auxiliary function. The resulting Cᴺ continuous function is approximated with very good accuracy using any high order method, and the final solution can be obtained by inverse mapping. A relatively higher accuracy is achieved with less number of basis functions without any domain discretization. The proposed method is implemented to approximate functions in 1-D and 2-D. The 2-D results show that the method is scalable to higher dimensions. All the results and analyses show the proposed technique can potentially be used in solving many physical problems including Kato’s cusp and special plasmonics. The choice of auxiliary function (η) plays a key role in the approximation, and the accuracy and the efficiency of the proposed method is defined by the auxiliary function. The method is also implemented to a simple ODE to show that the method is equally applicable to differential equations.

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