Generation of collocation points in the method of fundamental solutions for 2D Laplace’s equation

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Abstract
We propose a new method for generating collocation points that give an accurate approximation in the method of fundamental solutions (MFS). It is known that collocation points that maximize the determinant of the coefficient matrix of the linear system in the MFS give an accurate approximation. However, the maximization problem is intractable. We design an efficient algorithm to automatically take collocation points that do not depend on a boundary condition. Numerical experiments show that the proposed collocation points give a better condition number and an accurate approximation when we use source points far from the boundary.

Keywords method of fundamental solutions, collocation points, maximization of a determinant, second-order cone programming

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1. Introduction

The method of fundamental solutions (MFS) is a meshfree method for solving some partial differential equations. Some features of the MFS are the simplicity of its implementation, the speed of its calculation, and the accuracy under a certain condition. The accuracy of the MFS depends on the location of collocation points and source points. However, the problem of how to locate automatically and efficiently them to obtain an accurate solution has been an open question.

To deal with various boundary conditions, we focus on finding a method for giving collocation points that depend on a boundary shape, and not on a boundary condition. Some examples of the methods of giving such collocation points are provided by [1, 2]. Sugihara [3] proved that the collocation points that maximize the determinant of the coefficient matrix give an accurate approximation. However, the maximization problem is intractable. We create a tractable optimization problem for generating collocation points. It is a maximization problem of the determinant of the matrix that approximates the coefficient matrix of the linear system in the MFS.

This article is organized as follows. In Section 2, we present the problem that we examine, the fundamental of the MFS and the concept of generalized Fekete points introduced by Sugihara [3]. In Section 3, we present the process of introducing a new method. In Section 4, we show an optimization problem to solve and present an algorithm to obtain collocation points. In Section 5, we present numerical experiments that show the accuracy of the proposed method and the condition numbers of the coefficient matrix in the proposed method. In Section 6, we give some conclusions and future work.

2. Preliminaries

We consider the boundary value problem

$$\begin{aligned}
\Delta u &= 0 \quad \text{in } \Omega, \\
u &= f \quad \text{on } \partial \Omega,
\end{aligned}$$

where $\Omega \subset \mathbb{R}^2$ is a bounded simply connected region, $\partial \Omega$ is the boundary of $\Omega$, and $f$ is a given function. In the MFS, the solution $u$ is approximated by

$$u^{(N)}(x) = \sum_{k=1}^{N} Q_k E(x - y_k),$$

where $E(x) = \log |x|$, and $N$ points $y_1, \ldots, y_N \in \mathbb{R}^2$ lie outside $\Omega$. The points $y_1, \ldots, y_N$ are called the source points. The coefficients $Q_1, \ldots, Q_N \in \mathbb{R}$ are determined by the collocation method. Collocation points $x_1, \ldots, x_N \in \mathbb{R}^2$ are placed on $\partial \Omega$, and the following boundary conditions are imposed:

$$u^{(N)}(x_j) = f(x_j), \quad j = 1, \ldots, N.$$  

This yields a linear system which has the form

$$AQ = f,$$

where the elements of the matrix $A \in \mathbb{R}^{N \times N}$ are given by $A_{j,k} = E(x_j - y_k)$, $Q = (Q_1 \ldots Q_N)^\top \in \mathbb{R}^N$, and $f = (f(x_1) \ldots f(x_N))^\top \in \mathbb{R}^N$.

Generalized Fekete points in the MFS were introduced as collocation points that give an accurate approximate solution in [3]. They are defined as a solution to the following optimization problem:

$$\begin{aligned}
\text{maximize} & \quad | \det A |, \\
\text{subject to} & \quad x_1, \ldots, x_N \in \partial \Omega.
\end{aligned}$$
If we use Fekete points as collocation points in the MFS, the following inequality holds [3]:
\[
\max_{x \in \partial \Omega} \left| u(x) - u^{(N)}(x) \right| \leq (N + 1) \inf_{g \in \text{span} \{\psi_1, \ldots, \psi_N\}} \left( \max_{x \in \partial \Omega} \left| u(x) - g(x) \right| \right),
\]
where \( \psi_j(x) = E(x - y_j) \); that is, Fekete points give an accurate approximation. Nevertheless, the problem of how to efficiently solve the optimization problem (5) is an open question.

3. Determinant maximization

In this section, we present the process of introducing a new method. This section consists of two parts: first, we approximate the coefficient matrix to a product of the two matrices, one depends only on the collocation points and the other depends on only the source points; second, using discretization and the continuous relaxation, we approximate the optimization problem by a convex one.

We approximate the matrix \( A \) and formulate another easier optimization problem. Assume that
\[
\min_k |y_k| > \max_k |x_k|,
\]
that is, source points are far from the boundary. We approximate the matrix \( A \) with Fourier expansion of logarithmic function [4]. We expand it in the following way:
\[
\log |x - y| = \log r_y - \sum_{k=1}^{\infty} \frac{1}{k} \left( \begin{array}{c} r_x \\ r_y \end{array} \right)^k \cos(k \theta_x - \theta_y)
= \sum_{k=1}^{\infty} \varphi_k(x) \tilde{\varphi}_k(y),
\]
where \( r_x, \theta_x, r_y, \theta_y \) are the polar coordinates,
\[
\varphi_k(x(r_x, \theta_x)) = \begin{cases} \frac{1}{k} \cos \frac{k}{2} \theta_x & (k = 1), \\
\frac{1}{k} \cos \frac{k}{2} \theta_x \sin \frac{k-1}{2} \theta_x & (k = 2, 4, \ldots), \\
\frac{1}{k} \cos \frac{k}{2} \theta_x \sin \frac{k-1}{2} \theta_x & (k = 3, 5, \ldots),
\end{cases}
\]
\[
\tilde{\varphi}_k(y(r_y, \theta_y)) = \begin{cases} \log r_y & (k = 1), \\
\left( \frac{k}{2r_y} \right)^{-1} \cos \frac{k}{2} \theta_y & (k = 2, 4, \ldots), \\
\left( \frac{k}{2r_y} \right)^{-1} \sin \frac{k-1}{2} \theta_y & (k = 3, 5, \ldots).
\end{cases}
\]

With this expansion, we have \( A \approx BF \),
\[
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\]
where
\[
B := \begin{pmatrix} \tilde{\varphi}_1(y_1) & \ldots & \tilde{\varphi}_N(y_1) \\
\vdots & \ddots & \vdots \\
\tilde{\varphi}_1(y_N) & \ldots & \tilde{\varphi}_N(y_N) \end{pmatrix},
\]
\[
F := \begin{pmatrix} \varphi_1(x_1) & \ldots & \varphi_1(x_N) \\
\vdots & \ddots & \vdots \\
\varphi_N(x_1) & \ldots & \varphi_N(x_N) \end{pmatrix}
\]

With this expansion, we have \( \det A \approx \det B \det F \). Since \( B \) does not depend on the collocation points, we maximize \( \det F \) to maximize \( \det A \). Note that we can maximize \( \det A \) by maximizing \( \det A \) because interchanging two collocation points changes the sign of \( \det A \).

We approximately maximize \( \det F \) by convex optimization. We do not directly maximize \( \det F \); we maximize \( (\det F)^2 \). We set \( \varphi(x) := (\varphi_1(x) \ldots \varphi_N(x))^T \in \mathbb{R}^N \), and the maximization problem is represented as follows:
\[
\begin{aligned}
\text{maximize} & \quad \det \left( \sum_{k=1}^{N} \varphi(x_k) \varphi(x_k)^T \right), \\
\text{subject to} & \quad x_1, \ldots, x_N \in \partial \Omega.
\end{aligned}
\]

This maximization problem is known as a D-optimal design of experiments and NP-hard [5]. Therefore, we solve a continuous relaxation of the problem (15). We present it in the next section.

4. Proposed method

We consider the following optimization problem:
\[
\begin{aligned}
\text{maximize} & \quad \det \left( \sum_{k=1}^{M} w_k \varphi(x_k') \varphi(x_k')^T \right), \\
\text{subject to} & \quad \sum_{k=1}^{M} w_k = N, \quad w_1, \ldots, w_M \in \{0, 1\}.
\end{aligned}
\]

This maximization problem is known as a D-optimal design of experiments and NP-hard [5]. Therefore, we can efficiently solve the optimization problem (16).

By using the solution of Problem (16), we place \( N \) collocation points in the following way.

(1) Solve a Problem (16). (2) Pick points from \( \{x_k'\}_{k=1}^{M} \) corresponding to “local maxima” of \( \{w_k\}_{k=1}^{M} \).

(3) When the number of the picked points is larger than \( N \), pick the \( N \) points corresponding to the top \( N \) weights \( w_k \).

(4) Choose \( N \) collocation points as the picked \( N \) points. “Local maximum” of \( \{w_k\}_{k=1}^{M} \) means the component \( w_j \) satisfying \( w_j \geq w_k \) for any “neighbors” \( k \in \mathcal{N}_j := \{k \mid x_k' \text{ is a neighbor of } x'_j \in \partial \Omega \} \). We determine the neighbors of \( x'_j \) according to the distance on \( \partial \Omega \).
5. Numerical experiments

We present numerical experiments in order to show that the proposed collocation points give an accurate approximation. We did not examine a set of source points \( \{y_k\}_{k=1}^{N} \) in this article and uniformly assigned them on a circle such that the assumption (7) is satisfied. Note that source points are far from the boundary.

We carried out experiments by using MATLAB2016b and the MOSEK optimization toolbox for MATLAB 8.1.0.72 (https://www.mosek.com/, last accessed on 15 January 2019). We solved optimization problems (16) by reducing them to second-order cone programming problems [6, 7]. We used the mldivide function in MATLAB for solving the linear equation (4). We carried out all computations in double precision. It took a few minutes to generate collocation points by the proposed method in each case. The time for making the SOCP instance and solving it in the case of \( N = 70 \) and \( M = 700 \) (inside the curve (18)) was 233.73 seconds by a computer with Intel Xeon CPU E5-2620v4 2.10 GHz and 32 GB RAM.

We first consider the non-convex region surrounded by the following curve:

\[
\gamma(t) := (r(t) \cos(\pi t), r(t) \sin(\pi t)),
\]

where

\[
r(t) := \sqrt{\cos(2\pi t) + \sqrt{2 - \sin^2(2\pi t)}}.
\]

(17)

This boundary curve is called the Cassini oval. This type of region is dealt with in, for example, [2, 4]. Source points are determined by \( y_k = (5 \cos \theta_k, 5 \sin \theta_k) \), where \( \theta_k = (2k/N - 1) \pi, \ k = 1, \ldots, N \). In the maximization problem (16), \( M = 600 \), and \( x_k = \gamma(2k/M - 1), k = 1, \ldots, M \). We present the location of the collocation points given by the proposed method in the case of \( N = 40 \) in Fig. 1. We present the maximum errors for the harmonic boundary condition \( f(x, y) = e^x \cos y \) in Fig. 2 and for the nonharmonic boundary condition \( f(x, y) = \cos x - x^2 y \) in Fig. 3. We present the condition numbers of the coefficient matrices of the linear system (4) in Fig. 4. We compare the proposed arrangement of the collocation points with the following ones: the “Equal angle” collocation points \( x_k = \gamma(\theta_k) \), and the “Equal segments” collocation points splitting the boundary by equal length segments. As can be observed from Fig. 1, the collocation points chosen by the proposed method are densely distributed in the parts far from the origin. As can be observed from Fig. 2 and Fig. 3, the errors of the proposed arrangements are the least among those of the three arrangements in the two cases. As can be observed from Fig. 4, the proposed arrangements give the relatively better condition numbers.

We next consider the gear-shaped region surrounded by the following curve:

\[
\gamma(t) = (r(t) \cos \theta(t), r(t) \sin \theta(t)),
\]

where

\[
r(t) = 1 + \frac{\sin(7\pi t)}{4}, \ \theta(t) = \pi t + \frac{\sin(7\pi t)}{2},
\]

(18)

This type of region is dealt with in, for example, [8]. Source points are determined by \( y_k = (2 \cos \theta_k, 2 \sin \theta_k) \), where \( \theta_k = (2k/N - 1) \pi, \ k = 1, \ldots, N \). In the maximization problem (16), \( M = 700 \), and \( x_k = \gamma(2k/M - 1), k = 1, \ldots, M \). We present the location of the collocation points in the case of \( N = 63 \) in Fig. 5. We present the maximum errors for the boundary condition \( f(x, y) = x^2 - y^2 \) in Fig. 6. We present the condition numbers of the coefficient matrix of the linear system (4) in Fig. 7. We compare the proposed arrangement of the collocation points with the following ones: the “Equal parameter differences” collocation points \( x_k = \gamma(2k/N - 1), k = 1, \ldots, N \), and the “Equal segments” collocation points splitting the boundary by equal length segments. As can be observed from Fig. 5, the collocation points chosen by the proposed method...
are not located at the inner segments of the boundary, and they are densely distributed in the parts far from the origin. As can be observed from Fig. 6, the trends of the errors of the arrangements except for the proposed one do not continue for large $N$, and the errors of the proposed arrangements are the least in the case of large $N$. This seems to be owing to numerical stability. We observe from Fig. 7 that the condition numbers get worse as $N$ increases and that the proposed arrangements give the relatively better condition numbers. In nonharmonic boundary conditions, errors in the three arrangements did not get small as $N$ increased. Thus, in those cases, we must examine other arrangements of collocation points and source points.

6. Concluding remarks

We propose the method of maximizing the determinant of the matrix that approximates the coefficient matrix of the linear system in the MFS, and we obtain collocation points that give an accurate approximation. Some features of the proposed method are that collocation points are located automatically and efficiently, and that they depend on the boundary shape and not on the boundary condition. In the numerical experiments, when source points are located far from the boundary, our method gives relatively better condition number and an accurate approximation. Our method comes from theoretical consideration, but it does not have a theoretical error analysis, which is a topic for future work. The extension of this method to a higher dimension is also a topic for future work.

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