

An Efficient Least–Squares MFS Algorithm for Certain Harmonic Problems

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Abstract: *The Method of Fundamental Solutions (MFS) is a boundary–type meshless method for the solution of certain elliptic boundary value problems. In this work, we propose an efficient algorithm for the linear least–squares version of the MFS, when applied to the Dirichlet problem for Laplace equation in a disk.*

Keywords: Method of fundamental solutions, linear least–squares method, boundary meshless methods, elliptic boundary value problems.

1 Introduction

In the MFS, the solution is approximated by a linear combination of fundamental solutions of the operator of the partial differential equation of the problem under consideration. This approximation thus satisfies the differential equation and the coefficients in the linear combination are determined from the boundary conditions. The satisfaction of the boundary conditions can be done in two ways: One way is by fixing and preassigning the locations of the singularities and simply collocating the boundary conditions. This leads to a linear system with the same number of equations as unknowns or a linear least–squares problem. Alternatively, the locations of the singularities can be determined along with the coefficients, which results in a non–linear least–squares problem. Details and applications of these formulations can be found in the recent survey papers [2, 3, 5]. A description of the linear least–squares MFS can be found in Golberg and Chen [4] and Ramachandran [6]. In this paper, we consider the linear least–squares formulation of the problem.

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2 The linear least-squares MFS

We consider the boundary value problem

$$\begin{cases} Lu = 0 & \text{in } \Omega, \\ u = f & \text{on } \partial\Omega, \end{cases} \quad (2.1)$$

where L is a second order linear elliptic operator, Ω is an open bounded domain in \mathbb{R}^2 . In the MFS, the solution is approximated by

$$u_N(c, Q; P) = \sum_{j=1}^N c_j k(P, Q_j), \quad P \in \bar{\Omega}, \quad (2.2)$$

where $c = (c_1, c_2, \dots, c_N)^T$ and Q is a $2N$ -vector containing the coordinates of the singularities Q_j , $j = 1, \dots, N$, which lie on the boundary $\partial\Omega'$, of the domain Ω' , where $\bar{\Omega} \subset \Omega'$. The function $k(P, Q)$ is a fundamental solution of the elliptic operator L . The satisfaction of the boundary condition is imposed on a set of boundary points $\{P_i\}_{i=1}^M$:

$$u_N(c, Q; P_i) = f(P_i), \quad i = 1, \dots, M. \quad (2.3)$$

This yields the linear system $Gc = f$, where the elements of the matrix $G \in \mathbb{R}^{M \times N}$ are given by $g_{i,j} = k(P_i, Q_j)$, $i = 1, \dots, M$, $j = 1, \dots, N$. If $M > N$, we seek a least-squares solution of this system, i.e. the N coefficients c_1, \dots, c_N , which minimize the functional

$$\Phi(c_1, \dots, c_N) = \sum_{i=1}^M \left| \sum_{j=1}^N c_j k(P_i, Q_j) - f(P_i) \right|^2.$$

Therefore, these coefficients c_1, \dots, c_N must satisfy the *normal equations*

$$\frac{\partial}{\partial c_j} \Phi(c_1, \dots, c_N) = 0, \quad j = 1, \dots, N,$$

or equivalently

$$\sum_{i=1}^M k(P_i, Q_j) \left\{ \sum_{j=1}^N c_j k(P_i, Q_j) - f(P_i) \right\} = 0, \quad j = 1, \dots, N,$$

that is

$$G^* G c = G^* f, \quad (2.4)$$

where G^* is the transpose of G .

3 Efficient implementation

We consider the special case of Laplace's equation in the disk of radius ρ , i.e. $L = \Delta$ and $\Omega = B_\rho = \{x \in \mathbb{R}^2 : |x| < \rho\}$, with boundary $\partial\Omega = S_\rho = \{x \in \mathbb{R}^2 : |x| = \rho\}$. The fundamental solution k is given by $k(P, Q) = -\frac{1}{2\pi} \log |P - Q|$, with $|P - Q|$ denoting the distance between the points P and Q . The singularities Q_j^α are fixed on the boundary S_R of the disk B_R concentric to B_ρ , where $R > \rho$. A set of collocation points $\{P_i\}_{i=1}^M$, where $M \geq N$, is placed on S_ρ . If $P_i = (x_{P_i}, y_{P_i})$, then we take

$$x_{P_i} = \rho \cos \frac{2(i-1)\pi}{M}, \quad y_{P_i} = \rho \sin \frac{2(i-1)\pi}{M}, \quad i = 1, \dots, M.$$

The locations of the singularities, $Q_j^\alpha = (x_{Q_j^\alpha}, y_{Q_j^\alpha})$ are defined by

$$x_{Q_j^\alpha} = R \cos \left(\frac{2(j-1)\pi}{N} + \frac{2\alpha\pi}{M} \right), \quad y_{Q_j^\alpha} = R \sin \left(\frac{2(j-1)\pi}{N} + \frac{2\alpha\pi}{M} \right), \quad (3.1)$$

where $j = 1, \dots, N$. The positions of the singularities differ by an angle $\frac{2\pi\alpha}{M}$ from the positions of the boundary points and $0 \leq \alpha < 1$. The elements of the matrix G_α are given by $g_{i,j}^\alpha = -\frac{1}{2\pi} \log |P_i - Q_j^\alpha|$, $i = 1, \dots, M$, $j = 1, \dots, N$. In the case when M is an integer multiple of N , i.e. $M = mN$ with $m \in \mathbb{N}$, the matrix G_α has the form (dropping the α 's)

$$G_\alpha = \begin{pmatrix} g_{1,1} & g_{1,2} & \cdots & g_{1,N} \\ g_{2,1} & g_{2,2} & \cdots & g_{2,N} \\ \vdots & \vdots & & \vdots \\ g_{m,1} & g_{m,2} & \cdots & g_{m,N} \\ \hline g_{1,N} & g_{1,1} & \cdots & g_{1,N-1} \\ \vdots & \vdots & & \vdots \\ g_{m,N} & g_{m,1} & \cdots & g_{m,N-1} \\ \hline g_{1,N-1} & g_{1,N} & \cdots & g_{1,N-2} \\ \vdots & \vdots & & \vdots \\ g_{m,N-1} & g_{m,N} & \cdots & g_{m,N-2} \\ \hline \cdots \\ \hline g_{1,2} & g_{1,3} & \cdots & g_{1,1} \\ \vdots & \vdots & & \vdots \\ g_{m,2} & g_{m,3} & \cdots & g_{m,1} \end{pmatrix} \begin{array}{l} \text{row 1} \\ \text{row 2} \\ \vdots \\ \text{row } m \\ \hline \text{row } m+1 \\ \vdots \\ \text{row } 2m \\ \hline \text{row } 2m+1 \\ \vdots \\ \text{row } 3m \\ \hline \cdots \\ \hline \text{row } (N-1)m+1 \\ \vdots \\ \text{row } Nm \end{array}$$

We observe that row $m+1$ is a rotation of row 1, row $2m+1$ is a rotation of row $m+1$ and in general row $\mu m + \kappa$ is a $\mu - \nu$ rotation of row $\nu m + \kappa$ for $\kappa = 1, \dots, m$.

3.1 Diagonalization of the matrix $G_\alpha^* G_\alpha$

In order to achieve this, we must first examine the matrix $U_M G_\alpha U_N^*$, where $(U_N^*)_{kl} = \frac{1}{\sqrt{N}} \omega_N^{(k-1)(l-1)}$ with $\omega_N = e^{\frac{2\pi i}{N}}$. The matrix U_N is clearly unitary. If we set $h_j = g_{j,1}$, $j =$

$1, \dots, M$, and let λ_j , $j = 1, \dots, M$, be the eigenvalues of $H = \text{circ}(h_1, \dots, h_M)$ then we have the expression (see [1])

$$\lambda_j = \sum_{k=1}^M h_k \omega_M^{(j-1)(k-1)}. \quad (3.2)$$

The matrix $U_M G_\alpha$ is then

$$\frac{1}{\sqrt{M}} \begin{pmatrix} \bar{\lambda}_1 & \bar{\lambda}_1 & \bar{\lambda}_1 & \cdots & \bar{\lambda}_1 \\ \bar{\lambda}_2 & \bar{\omega}_M^m \bar{\lambda}_2 & \bar{\omega}_M^{2m} \bar{\lambda}_2 & \cdots & \bar{\omega}_M^{(N-1)m} \bar{\lambda}_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \bar{\lambda}_N & \bar{\omega}_M^{(N-1)m} \bar{\lambda}_N & \bar{\omega}_M^{2(N-1)m} \bar{\lambda}_N & \cdots & \bar{\omega}_M^{(N-1)(N-1)m} \bar{\lambda}_N \\ \bar{\lambda}_{N+1} & \bar{\lambda}_{N+1} & \bar{\lambda}_{N+1} & \cdots & \bar{\lambda}_{N+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \bar{\lambda}_{2N} & \bar{\omega}_M^{(2N-1)m} \bar{\lambda}_{2N} & \bar{\omega}_M^{2(2N-1)m} \bar{\lambda}_{2N} & \cdots & \bar{\omega}_M^{(N-1)(2N-1)m} \bar{\lambda}_{2N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \bar{\lambda}_{mN} & \bar{\omega}_M^{(mN-1)m} \bar{\lambda}_{mN} & \bar{\omega}_M^{2(mN-1)m} \bar{\lambda}_{mN} & \cdots & \bar{\omega}_M^{(N-1)(mN-1)m} \bar{\lambda}_{mN} \end{pmatrix};$$

that is, $(U_M G_\alpha)_{k,\ell} = \frac{1}{\sqrt{M}} \bar{\omega}_M^{m(k-1)(\ell-1)} \bar{\lambda}_k$, where $k = 1, \dots, M$ and $\ell = 1, \dots, N$. Post-multiplication of $U_M G_\alpha$ by U_N^* yields the $M \times N$ matrix

$$U_M G_\alpha U_N^* = \frac{1}{\sqrt{m}} \begin{pmatrix} \bar{\lambda}_1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \bar{\lambda}_2 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \bar{\lambda}_3 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \bar{\lambda}_{N-1} & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & \bar{\lambda}_N \\ \bar{\lambda}_{N+1} & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \bar{\lambda}_{N+2} & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \bar{\lambda}_{2N} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \bar{\lambda}_{mN} \end{pmatrix};$$

that is, $(U_M G_\alpha U_N^*)_{k,\ell} = \frac{1}{\sqrt{m}} \delta_{k,\ell}^N \bar{\lambda}_k$, where

$$\delta_{k,\ell}^N = \begin{cases} 1 & \text{if } k \equiv \ell \pmod{N} \\ 0 & \text{if } k \not\equiv \ell \pmod{N}. \end{cases}$$

Finally,

$$\begin{aligned} (U_M G_\alpha U_N^*)^* U_M G_\alpha U_N^* &= U_N G_\alpha^* U_M^* U_M G_\alpha U_N^* = U_N G_\alpha^* G_\alpha U_N^* \\ &= \text{diag}(\mu_1, \dots, \mu_N) := \Lambda, \end{aligned}$$

where

$$\mu_\ell = \frac{1}{m} \sum_{j=1}^m |\lambda_{(j-1)N+\ell}|^2. \quad (3.3)$$

The μ_ℓ , $\ell = 1, \dots, N$, are the eigenvalues of G^*G . We have thus obtained the diagonalization of $G_\alpha^*G_\alpha$:

$$G_\alpha^*G_\alpha = U_N^*\Lambda U_N. \quad (3.4)$$

The following theorem guarantees the solvability of (2.4).

Theorem 3.1. *For every $\alpha \in [-\frac{1}{2}, \frac{1}{2}]$ and $m \geq 2$, the matrix $G_\alpha^*G_\alpha$ is nonsingular.*

PROOF. This follows from Theorem 2.11 of [8] according to which the only possibly vanishing eigenvalues among the λ_j , $j = 1, \dots, M$, are

- (i) $\lambda_1(\alpha)$, which may occur only for $\alpha \in (-\frac{1}{6}, \frac{1}{6})$, and
- (ii) $\lambda_{M/2+1}(\frac{1}{2})$, if M is even.

Clearly, for $m = M/N \geq 2$, formula (3.3) shows that no eigenvalue μ_ℓ , $\ell = 1, \dots, N$, vanishes. \square

System (2.4) may be written as

$$U_N G_\alpha^* G_\alpha U_N^* U_N c = U_N G_\alpha^* U_M^* U_M f,$$

or equivalently,

$$\Lambda \hat{c} = \hat{G}_\alpha^* \hat{f}, \quad (3.5)$$

where $\hat{c} = U_N c$, $\hat{G}_\alpha^* = U_N G_\alpha^* U_M^*$ and $\hat{f} = U_M f$. Thus, if $\hat{f} = (\hat{f}_1, \dots, \hat{f}_M)$ and $\hat{c} = (\hat{c}_1, \dots, \hat{c}_N)$, the ℓ -th element of the vector $\hat{G}_\alpha^* \hat{f}$ is given by

$$(\hat{G}_\alpha^* \hat{f})_\ell = \frac{1}{\sqrt{m}} \sum_{j=1}^m \lambda_{(j-1)N+\ell} \hat{f}_{(j-1)N+\ell}, \quad (3.6)$$

where $\ell = 1, \dots, N$. Therefore, the solution of (3.5) is given by

$$\hat{c}_\ell = \sqrt{m} \frac{\sum_{j=1}^m \lambda_{(j-1)N+\ell} \hat{f}_{(j-1)N+\ell}}{\sum_{j=1}^m |\lambda_{(j-1)N+\ell}|^2}, \quad \ell = 1, \dots, N. \quad (3.7)$$

If we now let $k_j(P) = k(P, Q_j^\alpha)$, $j = 1, \dots, N$, and $k = (k_1(P), \dots, k_N(P))$, then (2.2) becomes

$$u_N(P) = \sum_{j=1}^N c_j k_j(P) = \langle c, k \rangle = \langle U_N c, U_N k \rangle = \langle \hat{c}, \hat{k} \rangle,$$

where $\langle \cdot, \cdot \rangle$ is the inner product in \mathbb{C}^N .

3.2 The algorithm

The following algorithm calculates the approximate solution (2.2):

Step 1 Compute $\hat{f} = U_M f$.

Step 2 Compute the eigenvalues $\lambda_j, j = 1, \dots, M$, from (3.2).

Step 3 Compute the vector \hat{c} from (3.7).

Step 4 Compute $\hat{k} = U_N k$.

Remarks 3.1.

- (i) *In Step 1, because of the form of the matrix U_M , the operation is equivalent to performing a Discrete Fourier Transform (DFT) of dimension M . This can be done at a cost of $O(M \log M)$ operations via an appropriate Fast Fourier Transform (FFT) algorithm. In Step 2, we first calculate the eigenvalues $\lambda_j, j = 1, \dots, M$, of the matrix $\text{circ}(h_1, \dots, h_M)$, at a cost of $O(M \log M)$ operations. Subsequently, we need an additional $O(M)$ operations to calculate the vector \hat{c} . In Step 3, the vector \hat{c} can be computed at a cost of $O(M)$ operations. Finally Step 4, can be carried out via inverse FFTs at a cost of $O(N \log N)$ operations. The total cost is therefore $O(M \log M)$.*
- (ii) *The efficient algorithm we propose is only applicable when the domain we are considering is a disk, but can be applied to different second-order elliptic operators with radial symmetry. For example, in the case of the Helmholtz equation*

$$\Delta u + \lambda^2 u = 0,$$

the fundamental solution is

$$k(P, Q) = -\frac{i}{4} H_0^{(2)}(\lambda |P - Q|),$$

where $H_0^{(2)}$ is the Hankel function of order 2. Clearly, the corresponding matrix $G_\alpha^ G_\alpha$ is also circulant.*

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