Optimization, conditioning and accuracy of radial basis function method for partial differential equations with nonlocal boundary conditions—A case of two-dimensional Poisson equation

Svajūnas Sajavičius*

Department of Computer Science II, Faculty of Mathematics and Informatics, Vilnius University, Naugarduko str. 24, LT-03225 Vilnius, Lithuania

Department of Mathematical Modelling, Faculty of Economics and Finance Management, Mykolas Romeris University, Ateities str. 20, LT-08303 Vilnius, Lithuania

Abstract

Various real-world processes usually can be described by mathematical models consisted of partial differential equations (PDEs) with nonlocal boundary conditions. Therefore, interest in developing computational methods for the solution of such nonclassical differential problems has been growing fast. We use a meshless method based on radial basis functions (RBF) collocation technique for the solution of two-dimensional Poisson equation with nonlocal boundary conditions. The main attention is paid to the influence of nonlocal conditions on the optimal choice of the RBF shape parameters as well as their influence on the conditioning and accuracy of the method. The results of numerical study are presented and discussed.

Keywords: Poisson equation, nonlocal boundary condition, meshless method, radial basis function, collocation, shape parameter, condition number

1. Introduction

Nonlocal boundary conditions arise in mathematical models of various physical, chemical, biological or environmental processes. For example, we can mention various problems arising in thermoelasticity, chemical diffusion or heat conduction processes, population dynamics and control theory. Related references and examples of mathematical models involving nonlocal boundary conditions can be found, for example, in paper [1].

In this paper, we consider the two-dimensional Poisson equation

$$\mathcal{L}[u] := -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f(x,y),\ 0 < x < 1,\ 0 < y < 1, \qquad (1)$$

subject to classical Dirichlet boundary conditions

$$u(0,y) = \mu_1(y), \quad 0 \le y \le 1, \qquad (2)$$

$$u(x,0) = \mu_3(x), \quad u(x,1) = \mu_4(x), \quad 0 \le x \le 1. \qquad (3)$$

Let us assume that on the boundary $x = 1$, a certain nonlocal boundary condition is formulated instead of classical boundary condition. In the present paper, we focus our attention on two examples of nonlocal boundary conditions:

- two-point condition

$$u(1,y) = \gamma u(\xi,y) + \mu_2(y), \quad 0 \le y \le 1, \qquad (4a)$$

- integral condition

$$u(1,y) = \gamma \int_{\xi_1}^{\xi_2} u(x,y)\mathrm{d}x + \mu_2(y), \quad 0 \le y \le 1. \qquad (4b)$$

Here $f(x,y)$, $\mu_1(y)$, $\mu_2(y)$, $\mu_3(x)$, $\mu_4(x)$ are given functions, γ, ξ ($0 \le \xi < 1$), ξ_1, ξ_2 ($0 \le \xi_1 < \xi_2 \le 1$) are given parameters (real numbers), and function $u(x,y)$ is unknown. We assume that boundary conditions (2)–(4) are compatible on the corners of the domain $[0,1]\times[0,1]$. The parameter γ can be interpreted as a measure of nonlocality. When $\gamma = 0$, we have a classical boundary-value problem, i.e., nonlocal boundary conditions (4a) and (4b) coincide with classical Dirichlet boundary condition $u(1,y) = \mu_2(y)$. If $\gamma \ne 0$, then nonlocal condition (4a) relates the values of unknown function on the boundary $x = 1$ with the values on the line $x = \xi$, and nonlocal integral condition (4b) relates the values of unknown function on the same boundary with the values on the interval $[\xi_1, \xi_2]$ by the term of definite integral respect to x.

In last decades, interest in developing numerical methods for the solution of partial differential equations (PDEs) with various types of nonlocal boundary conditions has been growing fast. Usually, finite difference, finite volume and finite element as well as various other traditional techniques are used (see, e.g., [1–15]).

*Correspondence address: Department of Computer Science II, Faculty of Mathematics and Informatics, Vilnius University, Naugarduko str. 24, LT-03225 Vilnius, Lithuania. Tel.: +370 5 2193091; fax: +370 5 2151585.

Email address: svajunas.sajavicius@mif.vu.lt svajunas@mruni.eu (Svajūnas Sajavičius)

URL: http://www.mif.vu.lt/~svajunas (Svajūnas Sajavičius)

doi:10.1016/j.enganabound.2013.01.009

In recent years, a lot of attention is paid to very attractive meshless (meshfree) methods for the numerical solution of PDEs [16–18]. The main advantage of meshless methods over the well-known mesh-based methods (such as finite differences, finite volumes, finite elements, etc.) is their geometrical flexibility. Meshless methods do not require mesh generation on the spatial domain of a problem. This advantage is important since mesh generation and remeshing are very expensive parts of the solution procedure, especially for two- or three-dimensional problems formulated on irregularly shaped domains [19].

One class of meshless methods are radial basis functions (RBF) collocation methods which use radial functions as the basis functions for the collocation. RBF are very efficient tools for the interpolation of a scattered multidimensional data as well as for the numerical solution of PDEs [20–23].

The standard RBF methods are based on the global interpolation. Certain RBF with successfully selected shape parameters and the usage of arbitrary precision arithmetics allow to achieve superior accuracy, even the exponential convergence rate is possible [24, 25]. In case of methods based on the local interpolation (such as finite element method), the convergence rate can be no better than algebraic (polynomial), which is very slow when high accuracy is necessary. The main disadvantage of the standard RBF technique is such that we must deal with dense (full) and, usually, ill-conditioned matrices. Nevertheless, in cases when accurate solutions of the problems formulated on complexly shaped multidimensional domains are desired, the RBF-based methods should be considered as useful alternative to traditional techniques.

In 1990, Kansa first time used Hardy's multiquadric (MQ) RBF [26] for the numerical solution of PDEs [27, 28]. Since then, RBF popularity in this area started to grow (see, e.g., [29–47] and some other references in the present paper). However, there are only few papers devoted to the RBF method for the solution of PDEs with nonlocal conditions. Probably the first time RBF method for the numerical solution of PDEs with nonlocal boundary conditions was used in paper [48]. RBF technique was tested for several problems with various types of nonlocal integral conditions and the results were compared with those obtained using the well-known finite difference schemes. In paper [49], an efficient collocation method for solving parabolic PDEs with nonlocal boundary conditions using RBF has been suggested. The RBF-based method for the one-dimensional wave equation with nonlocal integral condition has been proposed in paper [50]. A simple meshless RBF method for the solution of two-dimensional diffusion equation subject to Neumann's boundary conditions and nonlocal condition involving a double integral in a rectangular domain has been constructed in paper [51].

Above mentioned works [48–51] are mainly focused on demonstrating the efficiency of the RBF-based methods for the solution of one- and two-dimensional parabolic equations or one-dimensional hyperbolic (wave) equation with nonlocal boundary conditions. However, such questions as the influence of nonlocal boundary conditions on the optimal choice of the RBF shape parameters and their influence on the conditioning of the collocation matrix or the accuracy of the technique are not investigated yet.

The present paper is devoted to the RBF method for the solution of two-dimensional differential problem (1)–(4). To the best of our knowledge, this is the first time when RBF-based meshless method is used to solve a steady-state PDE (the two-dimensional Poisson equation) with nonlocal boundary condition. The main aim is to investigate the influence of nonlocal boundary conditions on the optimal choice of the RBF shape parameters as well as their influence on the conditioning and accuracy of the method. We test standard asymmetric collocation technique based on various types of RBF.

The paper is organized as follows. In Section 2, the basic definitions are given and the RBF method for the considered differential problem (1)–(4) is formulated. The results of numerical study (numerical experiments with several test problems) are presented and discussed in Section 3. Some remarks in Section 4 conclude the paper.

2. Construction of the method

2.1. Basic definitions

Let us recall standard definition of radial function. A multivariate real-valued function $\Phi : \mathbb{R}^d \to \mathbb{R}$ is called a *radial function* if there exists a univariate function $\phi : [0, \infty) \to \mathbb{R}$ such that

$$\Phi(\mathbf{x}) = \phi(\|\mathbf{x}\|),$$

where $\|\cdot\|$ is some norm on $\mathbb{R}^d$ (usually the Euclidean norm is used). Thus, the value $\Phi(\mathbf{x})$ depends only on the norm of vector $\mathbf{x}$.

In this paper, we will focus our attention on several types of RBF. The most popular globally supported and infinitely smooth RBF are listed in Table 1. All listed RBF contain a free parameter $\epsilon > 0$ which is called the shape parameter and controls the shape of the function. Usually, the shape parameter $c = 1/\epsilon$ is used in the expressions of RBF. Then, for example, MQ RBF is generated by function ϕ defined as $\phi(r) = \sqrt{c^2 + r^2}$.

Attention also will be paid to the generalized multiquadric (GMQ) RBF

$$\phi(r) = (1 + (\epsilon r)^2)^\beta,$$

where β is any real number except non-negative integers. The shape of GMQ RBF is controlled by two parameters (the exponent β and the shape parameter ϵ). It is clear that MQ, IMQ and IQ RBF are special cases of GMQ RBF with $\beta = 1/2, \beta = -1/2$

Table 1: Globally supported and infinitely smooth RBF ($r = \|\mathbf{x}\|$).

RBF	Definition
Multiquadric (MQ)	$\phi(r) = \sqrt{1 + (\epsilon r)^2}$
Inverse Multiquadric (IMQ)	$\phi(r) = (\sqrt{1 + (\epsilon r)^2})^{-1}$
Inverse Quadric (IQ)	$\phi(r) = (1 + (\epsilon r)^2)^{-1}$
Gaussian (GA)	$\phi(r) = \exp(-(\epsilon r)^2)$

and $\beta = -1$, respectively. GMQ RBF is much less investigated in comparison, for example, with MQ RBF.

When $\beta < 0$, GMQ RBF is strictly positive definite, while with $\beta > 0$ it is only conditionally positive definite of order $\lceil \beta \rceil$ [21, 22]. Therefore, IMQ and IQ RBF are strictly positive definite and MQ RBF is conditionally positive definite of order one. GA RBF also is strictly positive definite. For interpolation problem, the positive definiteness of RBF ensures the non-singularity (invertibility) of the interpolation matrix [52]. In case of conditionally positive definite RBF, the non-singularity of the problem is ensured by augmenting the interpolant with a polynomial of the corresponding order and appending some additional homogeneous linear equations to the interpolation system. Nevertheless, singular cases are very rare and interpolation based on conditionally positive RBF and without any augmentation of the interpolants are useful and efficient in practice.

For further theoretical details see, for example, [21, 22].

2.2. The method

When a meshless method is used for the solution of a steady-state differential problem, the spatial domain and its boundary are represented by a set of scattered points (nodes) [17]. In case of the RBF method, nodes traditionally are called centers (nodes coincide with the centers of RBF). Let

$$\Xi = \{(x_i, y_i)\}_{i=1}^N \subset [0,1] \times [0,1]$$

be a set of distinct scattered nodes which represent the spatial domain $[0,1]\times[0,1]$. We assume that $\Xi = \Xi_1 \cup \Xi_2 \cup \Xi_3 \cup \Xi_4 \cup \Xi_5$, where

$$\begin{aligned}
\Xi_1 &= \{(x_i, y_i) \in \Xi : 0 < x_i < 1, 0 < y_i < 1\},\\
\Xi_2 &= \{(x_i, y_i) \in \Xi : x_i = 0, 0 < y_i < 1\},\\
\Xi_3 &= \{(x_i, y_i) \in \Xi : x_i = 1, 0 < y_i < 1\},\\
\Xi_4 &= \{(x_i, y_i) \in \Xi : 0 \le x_i \le 1, y_i = 0\},\\
\Xi_5 &= \{(x_i, y_i) \in \Xi : 0 \le x_i \le 1, y_i = 1\},
\end{aligned}$$

and $\Xi_l \neq \emptyset$, $l = 1, 2, 3, 4, 5$.

Using the standard RBF interpolation approach, we seek for an approximate solution to the problem (1)–(4) in the form

$$\overline{u}(x, y) = \sum_{i=1}^N \lambda_i \phi_i(x, y),$$

where $\phi_i(x, y) = \phi(\|(x, y) - (x_i, y_i)\|_2)$ for a given RBF ϕ and center $(x_i, y_i) \in \Xi$, $\|\cdot\|_2$ denotes the Euclidean norm, and λ_i are coefficients to be determined using collocation technique.

Approximate solution $\overline{u}(x, t)$ imposed to satisfy the differential problem (1)–(4). Therefore, we have the following system of linear collocation equations:

$$\sum_{i=1}^N \lambda_i \mathcal{L}[\phi_i](x, y) = f(x, y), \quad (x, y) \in \Xi_1, \tag{5}$$

$$\sum_{i=1}^N \lambda_i \phi_i(x, y) = \mu_1(y), \quad (x, y) \in \Xi_2, \tag{6}$$

$$\sum_{i=1}^N \lambda_i (\phi_i(x, y) - \gamma I_i(y)) = \mu_2(y), \quad (x, y) \in \Xi_3, \tag{7}$$

$$\sum_{i=1}^N \lambda_i \phi_i(x, y) = \mu_3(x), \quad (x, y) \in \Xi_4, \tag{8}$$

$$\sum_{i=1}^N \lambda_i \phi_i(x, y) = \mu_4(x), \quad (x, y) \in \Xi_5, \tag{9}$$

where

$$I_i(y) = \phi_i(\xi, y) \quad \text{or} \quad I_i(y) = \int_{\xi_1}^{\xi_2} \phi_i(x, y) \mathrm{d}x$$

correspond to nonlocal parts of conditions (4a) or (4b), respectively.

For the functions ϕ listed in Table 1, computing of $I_i(y)$ is not complicated both in cases of conditions (4a) and (4b). Even in case of integral condition (4b), numerical integration is not required. Expressions of integrated (with respect to x) functions $\Phi(x, y) = \phi(\|(x, y)\|_2)$ are listed in Table 2. When GMQ RBF are used, nonlocal parts of conditions (4a) and (4b) are expressed as

$$I_i(y) = [1 + \epsilon^2((\xi - x_i)^2 + (y - y_i)^2)]^\beta$$

and

$$I_i(y) = \int_{\xi_1}^{\xi_2} [1 + \epsilon^2((x - x_i)^2 + (y - y_i)^2)]^\beta \mathrm{d}x, \tag{10}$$

respectively. According to Chebyshev theorem on the integration of binomial differentials, the indefinite integral of GMQ RBF (a special case of the binomial differential) with respect to x cannot be expressed in terms of elementary functions for any rational β, except in the cases where β or $\beta + 1/2$ is an integer. Therefore, in order to compute the integrals (10), usually it is necessary to apply a numerical integration procedure. In case of more general nonlocal boundary condition, such as

$$u(1, y) = \int_{\xi_1}^{\xi_2} \gamma(x) u(x, y) \mathrm{d}x + \mu_2(y), \quad 0 \le y \le 1,$$

where $\gamma(x)$ is given function, in order to compute the values

$$I_i(y) = \int_{\xi_1}^{\xi_2} \gamma(x) \phi_i(x, y) \mathrm{d}x,$$

numerical integration might be necessary even MQ, IMQ, IQ or GA RBF are used. It is possible to get explicit expressions of $I_i(y)$ for polynomial functions $\gamma(x)$ (this can be easily done using a computer algebra system).

Table 2: Expressions of integrated (with respect to x) functions $\Phi(x, y) = \phi(r)$ ($r = \|(x, y)\|_2$).

RBF	Integrated function
Multiquadric (MQ)	$\frac{1}{2}\left(x\sqrt{1+(\epsilon r)^2} + \frac{1+(\epsilon y)^2}{\epsilon} \cdot \ln\left(\epsilon x + \sqrt{1+(\epsilon r)^2}\right)\right)$
Inverse Multiquadric (IMQ)	$\frac{1}{\epsilon} \ln\left(\epsilon x + \sqrt{1+(\epsilon r)^2}\right)$
Inverse Quadric (IQ)	$\frac{1}{\epsilon\sqrt{1+(\epsilon y)^2}} \arctan\left(\frac{\epsilon x}{\sqrt{1+(\epsilon y)^2}}\right)$
Gaussian (GA)	$\frac{\sqrt{\pi}}{2\epsilon} \operatorname{erf}(\epsilon x) \exp\left(-(\epsilon y)^2\right)$

Thus, in order to determine unknown coefficients λ_i, we need to solve the linear system (5)–(9) which can be written in the matrix form as

$$\mathbf{A}\boldsymbol{\lambda} = \mathbf{b} \tag{11}$$

where $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_N)^T$ is unknown vector and $\mathbf{b}$ consists of the right-hand sides of linear equations (5)–(9). If globally supported RBF are used, then the matrix $\mathbf{A}$ is dense (full). Moreover, it tends to be very ill-conditioned when the shape parameter $\epsilon \to 0$ (and the exponent β is fixed, in case of GMQ RBF). The shape parameter ϵ also controls the accuracy of the method. In order to get accurate results, a small value of the shape parameter ϵ is required. Consequently, the method cannot be well-conditioned and very accurate at the same time. This is known as uncertainty (or trade-off) principle [22, 53].

We use the standard formulation of the RBF method. However, it is possible to use various approaches for the purpose of improving the method. For example, we can mention various techniques for improving the conditioning and accuracy of the MQ RBF asymmetric collocation method for elliptic PDEs [54], collocation both the boundary condition and PDE at the boundary points [55], Contour-Padé algorithm [56], usage of integrated MQ RBF [57] and a variable shape parameter (a different value of the shape parameter ϵ at each center) [27, 58, 59], RBF-QR method [60]. In order to get clear understanding about the influence of nonlocal boundary conditions on the properties of the method, none of these improvements were used in our study.

3. Numerical study

3.1. Technical details

In order to demonstrate the efficiency of the considered numerical method and investigate the influence of nonlocal boundary conditions on various properties of the method, several test problems were analyzed. In this paper, we present the results of numerical experiments with three test examples. In our examples, functions $f(x, y)$, $\mu_1(y)$, $\mu_2(y)$ and $\mu_3(x)$, $\mu_4(x)$ (initial data) were chosen so that particular functions $u(x, y)$ would be solutions to the differential problem (1)–(4). All these functions are listed in Table 3 and the graphs of functions $u(x, y)$ are plotted in Fig. 1.

On the problem domain, the nodes (centers of RBF) were distributed uniformly (see Fig. 2). Set Ξ consisted of $(\sqrt{N}-2)^2$ interior nodes ($|\Xi_1| = (\sqrt{N}-2)^2$) and $4(\sqrt{N}-1)$ nodes located on the boundary ($|\Xi_2| = |\Xi_3| = \sqrt{N}-2$, $|\Xi_4| = |\Xi_5| = \sqrt{N}$).

Table 3: The exact solutions and initial data of the test examples.

Test 1	
$u(x, y)$	$\exp(x+y)$
$f(x, y)$	$-2\exp(x+y)$
$\mu_1(y)$	$\exp(y)$
$\mu_2(y)$ [(4a)]	$\exp(1+y) - \gamma\exp(\xi+y)$
$\mu_2(y)$ [(4b)]	$\exp(1+y) - \gamma(-\exp(\xi_1+y) + \exp(\xi_2+y))$
$\mu_3(x)$	$\exp(x)$
$\mu_4(x)$	$\exp(x+1)$
Test 2	
$u(x, y)$	$\cos(\pi x)\cos(\pi y)$
$f(x, y)$	$2\pi^2\cos(\pi x)\cos(\pi y)$
$\mu_1(y)$	$\cos(\pi y)$
$\mu_2(y)$ [(4a)]	$-\cos(\pi y) - \gamma\cos(\pi\xi)\cos(\pi y)$
$\mu_2(y)$ [(4b)]	$-\cos(\pi y) + \gamma\cos(\pi y)(\sin(\pi\xi_1) - \sin(\pi\xi_2))/\pi$
$\mu_3(x)$	$\cos(\pi x)$
$\mu_4(x)$	$-\cos(\pi x)$
Test 3	
$u(x, y)$	$\sin(\pi x)\sin(\pi y)$
$f(x, y)$	$2\pi^2\sin(\pi x)\sin(\pi y)$
$\mu_1(y)$	0
$\mu_2(y)$ [(4a)]	$-\gamma\sin(\pi\xi)\sin(\pi y)$
$\mu_2(y)$ [(4b)]	$-\gamma\sin(\pi y)(\cos(\pi\xi_1) - \cos(\pi\xi_2))/\pi$
$\mu_3(x)$	0
$\mu_4(x)$	0

The examined meshless method has been implemented using Python programming language [61]. In case of GMQ RBF, the values of integrals (10) were computed using general purpose integration routine `quad` from SciPy subpackage `integrate`. Routine `quad` uses a technique (adaptive quadrature) from the Fortran library QUADPACK [62]. Linear systems (11) were solved using standard routine `solve` from SciPy subpackage `linalg`. SciPy package is built using the optimized ATLAS LAPACK and BLAS libraries [62]. The condition number of the matrix $\mathbf{A}$ was evaluated as the ratio of the largest and smallest singular values of $\mathbf{A}$,

$$\kappa(\mathbf{A}) = \|\mathbf{A}\|_2\|\mathbf{A}^{-1}\|_2 = \frac{\sigma_{\max}}{\sigma_{\min}}.$$

This ratio was computed using standard routines from SciPy package.

To estimate the accuracy of the numerical solution, we computed the max error

$$E_\infty = \max_{i=1,2,\ldots,N} |u(x_i, y_i) - \overline{u}(x_i, y_i)|,$$

and the root mean square (RMS) error

$$E_{\mathrm{RMS}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(u(x_i, y_i) - \overline{u}(x_i, y_i)\right)^2}.$$

Additional technical details of the numerical experiments will be specified later.

3.2. Results and discussion

3.2.1. Optimized values of the RBF shape parameters

Many popular RBF such as MQ, IMQ, IQ and GA contain a free parameter which controls the shape of the function. This parameter also has a strong influence on the conditioning and accuracy of the method. From Figs. 3 and 4 we can see how the

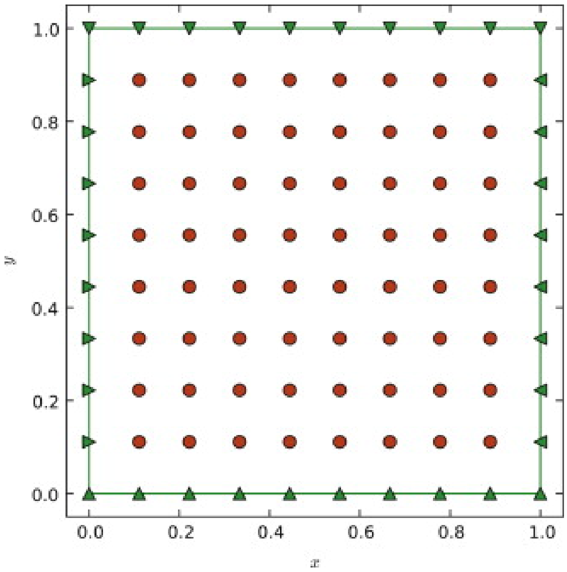

Figure 2: Representation of the domain $[0, 1] \times [0, 1]$ by uniformly distributed nodes ($N = 100$). Nodes from sets Ξ_1, Ξ_2, Ξ_3, Ξ_4 and Ξ_5 are marked as bullets (●), right-triangles (►), left-triangles (◄), up-triangles (▲) and down-triangles (▼), respectively.

conditioning and accuracy of the method depend on the values of the shape parameter ϵ when MQ RBF are used for the solution of the problem (1)–(4) with particular values of γ, ξ or ξ_1 and ξ_2. The minimal values of the errors E_∞ and $E_{\rm RMS}$ in all three cases are unstable (it is difficult to identify the optimal values of the shape parameter ϵ exactly). The region of such values of the shape parameter which lead to quite accurate results is limited. In case of each particular RBF and distribution of the nodes, the condition number of the matrix $\mathbf{A}$ depends on the shape parameter and the parameter γ of nonlocal boundary condition. We see that the method become ill-conditioned and lose its accuracy if the shape parameter is selected improperly. Thus, the selection of such value of the shape parameter which gives the most accurate results is very important and, unfortunately, very difficult problem.

The shape of GMQ RBF, as well as the conditioning and accuracy of the corresponding method, is controlled by the parameters β and ϵ. From Figs. 5 and 6 we see how the conditioning and accuracy of the method depend on the values of the exponent β when GMQ RBF with several different values of the shape parameter ϵ are used for the solution of the problem (1)–(4) with particular parameters of nonlocal condition. It is difficult to identify exactly which values of β give the most accurate results.

The first two ad hoc criteria for "optimal" shape parameter selection were proposed by Hardy [26] and Franke [63]. Rippa [64] suggested to use the leave-one-out cross validation (LOOCV) algorithm, which was extended by Fasshauer and Zhang [65] more recently. Various other strategies also have been suggested (for example, see [66–68]).

Recently, the problem of the optimal choice of the RBF shape parameters still remains very important and open. In paper [69], the influence of the shape parameter in the Gaussian radial basis function finite difference (RBF-FD) method with irregular centers on the quality of the approximation of the Dirichlet problem for the Poisson equation with smooth solution has been investigated and a multilevel algorithm that effectively finds a near-optimal shape parameter has been suggested. A novel algorithm for the shape parameter selection, based on a convergence analysis, is presented in paper [70]. Some results on the influence of the shape parameter in the error estimate of Gaussian interpolation have been obtained in paper [71]. An interesting numerical study exhibiting the role of the GMQ RBF shape parameters for the solution of elliptic PDEs is presented in paper [72]. In papers [73–75], various theoretical conjectures are explored using arbitrary precision computation. Finally, it should be noted that, in order to optimize the shape parameter, the residual error can be used as an error indicator [76].

For testing purposes, when the exact solution of the problem is known, trial and error method for the optimization of the shape parameters can be quite efficient. We used this technique when investigated the influence of nonlocal boundary conditions on the optimal values of the RBF shape parameters. For each test problem, we examined our method with values of the shape parameter ϵ (in case of MQ, IMQ, IQ and GA RBF) or the parameters β and ϵ (in case of GMQ RBF) obtained from random samples. In numerical experiments with MQ, IMQ, IQ and GA RBF, each sample consisted of 1000 random numbers uniformly distributed on the interval $(0, 10.0]$. When examined the method based on GMQ RBF, we used samples consisted of 10 000 pairs (β, ϵ), where β and ϵ were random numbers uniformly distributed on the intervals $(-10.0, 10.0]$ and $(0.0, 10.0]$, respectively. The values of the shape parameters which give the most accurate results for a fixed distribution and number of centers are assumed to be the optimized (near-optimal).

First of all, we investigated how the optimized values of the shape parameters depend on the values of γ. The values of γ were taken from samples of random numbers uniformly distributed on the interval $[-100.0, 100.0)$ (each sample consisted of 2000 random numbers). The values of parameter ξ (in case of condition (4a)) or parameters ξ_1 and ξ_2 (in case of condition (4b)) as well as the number of centers N were fixed.

The means and coefficients of variation (ratios of the standard deviations to the means, CV) of the optimized MQ, IMQ, IQ and GA RBF shape parameter ϵ are presented in Table 4. In case of Test 1, the coefficients of variation are smaller or approximately equal to 0.1. Slightly higher variances are observable in Test 2 and Test 3. In case of Test 3, the coefficients of variation are greater than 0.2 for both cases of nonlocal conditions (4a) and (4b). Nevertheless, all the coefficients of variation are greatly less than 1, i.e., variances are low. Thus, in all considered cases the variability of the optimized values of the shape parameter ϵ respect to the values of γ is low.

Since the optimized values of the exponent β can be both positive and negative, the variability of the optimized values of the GMQ RBF shape parameters is measured using the standard deviation (SD). From Table 5 we see that the variability of the optimized values of the parameter β is high, especially in cases of Test 2 and Test 3. In case of Test 3, the averaged optimized values of the parameter β are negative.

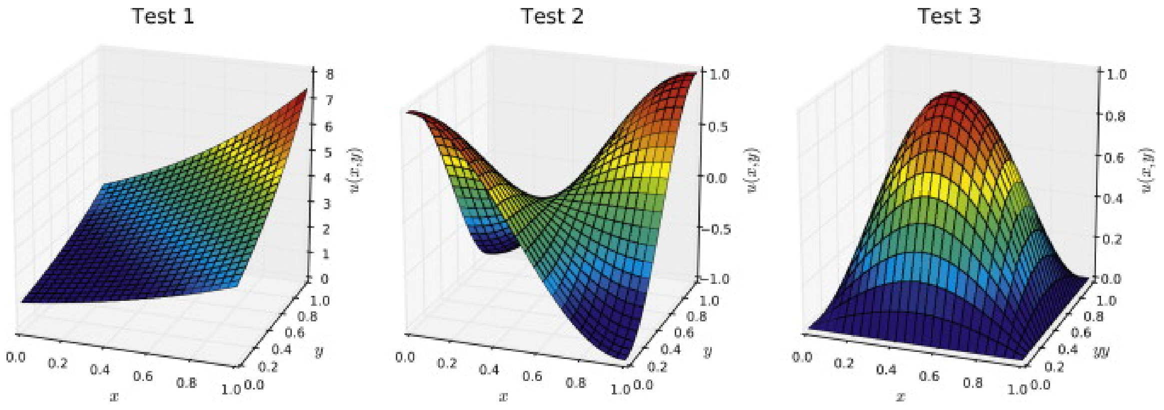

Figure 1: Plots of the exact solutions $u(x, y)$ of the test examples.

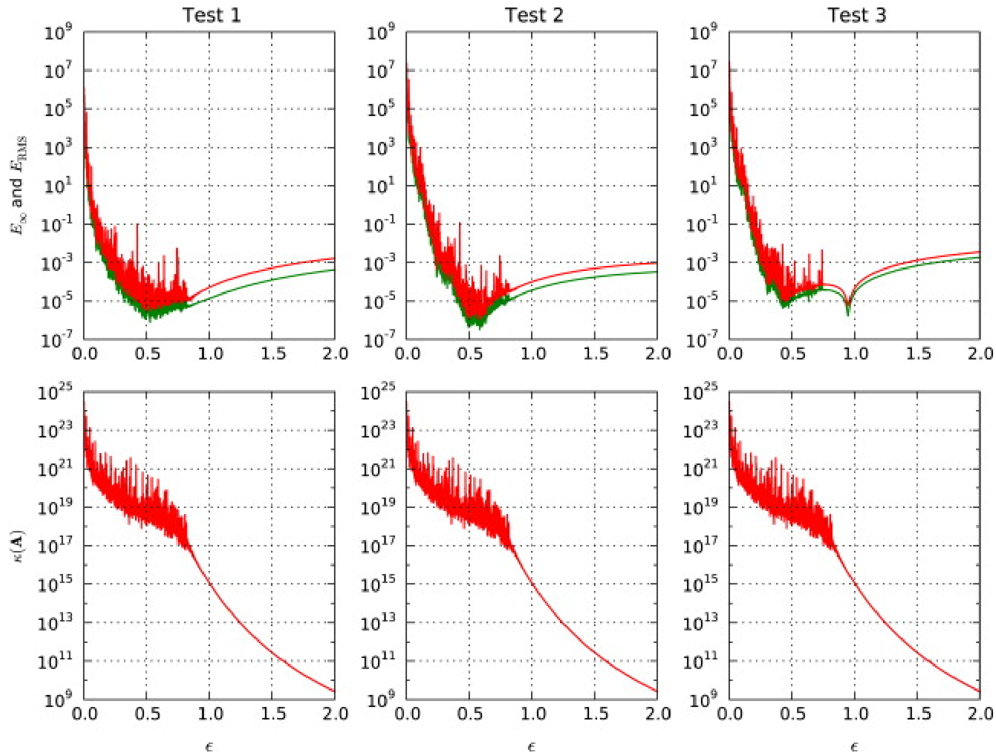

Figure 3: The dependence of the accuracy of the method (errors E_∞ and E_{RMS} are depicted as red curves and green curves, respectively) and the condition number $\kappa(\mathbf{A})$ (all three graphs in the second line represent the same data) on the values of MQ RBF shape parameter ϵ: problem with nonlocal boundary condition (4a), $\gamma = 1.0$, $\xi = 0.5$, $N = 100$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

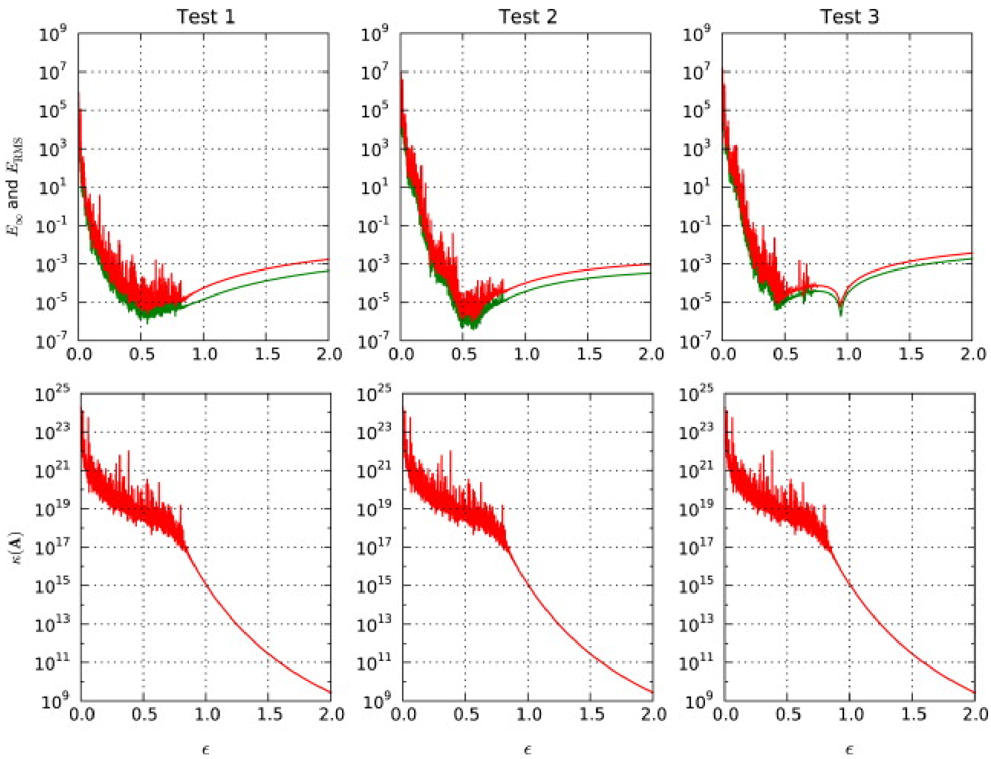

Figure 4: The dependence of the accuracy of the method (errors E_∞ and $E_{\rm RMS}$ are depicted as red curves and green curves, respectively) and the condition number $\kappa(\mathbf{A})$ (all three graphs in the second line represent the same data) on the values of MQ RBF shape parameter ϵ: problem with nonlocal condition (4b), $\gamma = 1.0$, $\xi_1 = 0.0$, $\xi_2 = 1.0$, $N = 100$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

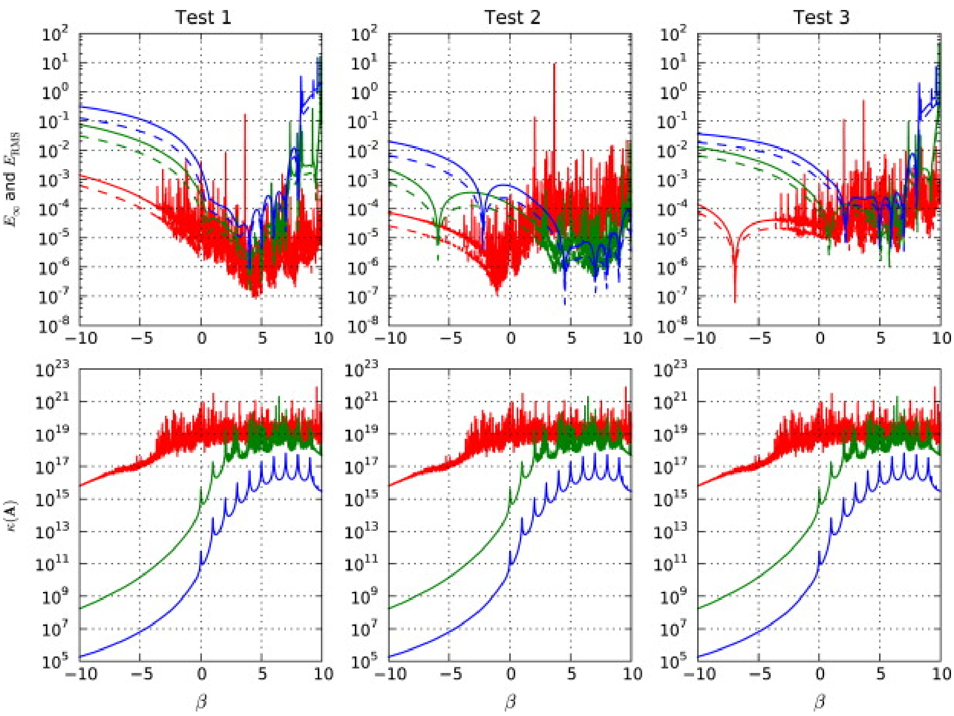

Figure 5: The dependence of the accuracy of the method (errors E_∞ and $E_{\rm RMS}$ are depicted as solid curves and dashed curves, respectively) and the condition number $\kappa(\mathbf{A})$ (all three graphs in the second line represent the same data) on the values of the GMQ RBF parameter β: problem with nonlocal boundary condition (4a), $\gamma = 1.0$, $\xi = 0.5$, $\epsilon = 0.5$ (red lines), $\epsilon = 1.0$ (green lines), $\epsilon = 1.5$ (blue lines), $N = 100$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

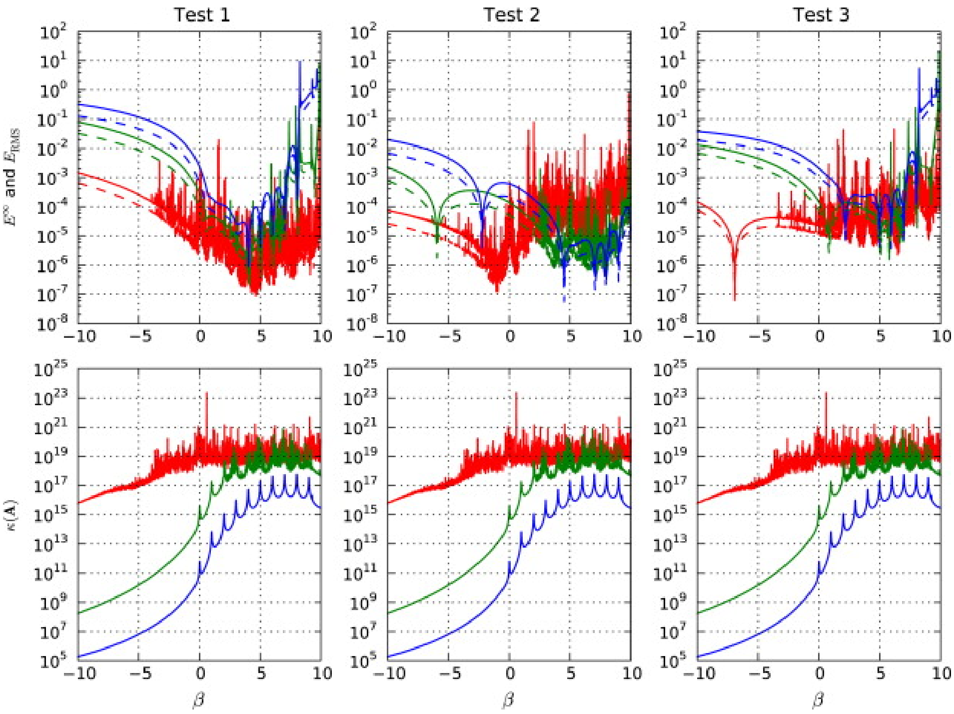

Figure 6: The dependence of the accuracy of the method (errors E_∞ and $E_{\rm RMS}$ are depicted as solid curves and dashed curves, respectively) and the condition number $\kappa(\mathbf{A})$ (all three graphs in the second line represent the same data) on the values of the GMQ RBF parameter β: problem with nonlocal boundary condition (4b), $\gamma = 1.0$, $\xi_1 = 0.0$, $\xi_2 = 1.0$, $\epsilon = 0.5$ (red lines), $\epsilon = 1.0$ (green lines), $\epsilon = 1.5$ (blue lines), $N = 100$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

Table 4: Means and coefficients of variation of the optimized values of the MQ, IMQ, IQ and GA RBF shape parameter ϵ: ξ or ξ_1 and ξ_2 were fixed ($\xi = 0.5$ or $\xi_1 = 0.0$ and $\xi_2 = 1.0$), γ was taken from random samples, $N = 100$.

		MQ	IMQ	IQ	GA
Problem with nonlocal condition (4a)					
Test 1					
Min. E_∞	Mean	0.570948630707	0.434771119978	0.382037142193	0.774627630899
	CV	0.0857715217498	0.0842158864327	0.0968117334031	0.0923498422023
Min. $E_{\rm RMS}$	Mean	0.572668648953	0.438794384611	0.385113021877	0.774722196781
	CV	0.0812766278521	0.082311949162	0.0921473442284	0.0863009864895
Test 2					
Min. E_∞	Mean	0.561844192351	0.519610104984	0.498482220599	1.20223542971
	CV	0.223356264589	0.239076730354	0.174628962207	0.0792320204078
Min. $E_{\rm RMS}$	Mean	0.557606978885	0.520756514295	0.499646599682	1.21031640864
	CV	0.0897045515829	0.248672728036	0.169912646503	0.0717629637452
Test 3					
Min. E_∞	Mean	0.868731949771	0.707721121403	0.604651229144	1.03141068628
	CV	0.216831126855	0.285044802302	0.350472114772	0.261856791374
Min. $E_{\rm RMS}$	Mean	0.863977270991	0.697756478368	0.591685855475	1.01866706478
	CV	0.221754216432	0.29516637622	0.360156839901	0.252803761724
Problem with nonlocal condition (4b)					
Test 1					
Min. E_∞	Mean	0.566374305499	0.445553885934	0.380367358006	0.775173935504
	CV	0.0920678790775	0.0952778466654	0.100472230068	0.0949217059922
Min. $E_{\rm RMS}$	Mean	0.569904069897	0.44915912783	0.383872160877	0.777298401682
	CV	0.0858438738256	0.0886332514393	0.0952858361182	0.0864950530324
Test 2					
Min. E_∞	Mean	0.565751987365	0.525277979221	0.49698715429	1.20140806046
	CV	0.224332906615	0.250849827133	0.11365465002	0.0861426219789
Min. $E_{\rm RMS}$	Mean	0.559963698542	0.518930339289	0.495791021342	1.20375360355
	CV	0.090152094309	0.193513434273	0.109725795822	0.0771095409975
Test 3					
Min. E_∞	Mean	0.852251891852	0.72189901672	0.622993148112	1.06962912608
	CV	0.228313188184	0.262292522147	0.33165204197	0.279203965992
Min. $E_{\rm RMS}$	Mean	0.850522282652	0.700611768727	0.603679742388	1.03990304786
	CV	0.233023886909	0.286613430494	0.347877101132	0.26644028703

Table 5: Means and standard deviations of the optimized values of the GMQ RBF shape parameters β and ϵ: ξ or ξ_1 and ξ_2 were fixed ($\xi = 0.5$ or $\xi_1 = 0.0$ and $\xi_2 = 1.0$), γ was taken from random samples, $N = 100$.

		β	ϵ
Problem with nonlocal boundary condition (4a)			
Test 1			
Min. E_∞	Mean	5.06903291227	0.597918707732
	SD	1.03144393384	0.29868056132
Min. E_{RMS}	Mean	4.94159242959	0.637608347473
	SD	0.878243700011	0.365721353381
Test 2			
Min. E_∞	Mean	3.87493708756	1.76769037639
	SD	3.78366858407	0.723917669832
Min. E_{RMS}	Mean	2.94598010763	1.59338189686
	SD	4.59455893161	0.658539913348
Test 3			
Min. E_∞	Mean	−3.04409551436	0.483585764739
	SD	5.79361332398	0.223979081057
Min. E_{RMS}	Mean	−2.97450622269	0.489652384922
	SD	5.92527015107	0.218338808473
Problem with nonlocal boundary condition (4b)			
Test 1			
Min. E_∞	Mean	4.94484099131	0.624647511577
	SD	0.804553650398	0.35386338254
Min. E_{RMS}	Mean	4.78945512753	0.679743673747
	SD	0.641447774178	0.409613199312
Test 2			
Min. E_∞	Mean	1.78600867657	1.41977498537
	SD	5.28101345705	0.706705494109
Min. E_{RMS}	Mean	0.781098331798	1.27079175584
	SD	5.60118553927	0.716372843041
Test 3			
Min. E_∞	Mean	−4.78775187572	0.507411216368
	SD	4.34188956112	0.168041524057
Min. E_{RMS}	Mean	−4.70683133432	0.517554226246
	SD	4.41030596905	0.164158949495

The influence of the location of parameter ξ or parameters ξ_1 and ξ_2 on the optimal selection of the shape parameters was also investigated. The value of γ was fixed while the values of parameter ξ or parameters ξ_1 and ξ_2 ($\xi_1 < \xi_2$) were taken from random samples (each sample consisted of 1000 random numbers uniformly distributed on the unit interval). For each particular value of ξ or pair (ξ_1, ξ_2), the above described trial and error procedure of the shape parameters optimization was executed.

The results obtained using MQ, IMQ, IQ and GA RBF are presented in Table 6. We see that variances are low in all considered cases. In cases of Test 1 and Test 2, the coefficients of variation are less than 0.1 while in case of Test 3 these coefficients are only slightly greater. Overall, the coefficients of variation are greatly less than 1, i.e., the variability of the optimized values of the RBF shape parameter ϵ respect to the values of ξ or ξ_1 and ξ_2 also is low.

However, from Table 7 we see that in case of Test 2 the variability of the optimized values of the exponent β in GMQ RBF respect to the values of ξ or ξ_1 and ξ_2 is high. The averaged optimized values of the parameter β are negative in cases of Test 2 and Test 3.

It should be noted that the optimal values of the shape parameters depend on the problem and on a total number of centers N. From Figs. 7 and 8 we see how the optimized values of the MQ, IMQ, IQ or GA RBF shape parameter ϵ depend on the number of centers N. It is known that the optimal values of the shape parameter ϵ also depend on the distribution of centers and on the precision of the computation [64].

From the results presented in the next subsection we will see that if the optimized (near-optimal) values of the shape parameters are used, the accuracy of the results is quite high in all considered cases.

3.2.2. *Conditioning and accuracy of the method*

The matrix of linear system (11) tends to be ill-conditioned if the shape parameter ϵ is decreased. Therefore, it could be difficult to obtain accurate solution of the linear system. To overcome this challenge, various approaches have been suggested (see, e.g., [19, 54, 77]). Recently, through numerical experiments, the condition numbers of the interpolation matrix for many species of RBF were examined in paper [78].

We investigated the influence of nonlocal conditions on the condition number of the collocation matrix $\mathbf{A}$ and the accuracy of the method. We solved differential problems with different values of γ, evaluated the condition number of the matrix $\mathbf{A}$ and computed the max and RMS errors. The number of centers was fixed ($N = 100$) and the averaged optimized values of the RBF shape parameter ϵ (see Table 4) were used.

The results of computations using MQ RBF are presented in Figs. 9 and 10. We note that in spite of high condition numbers, the accuracy of the method in cases of Test 1 and Test 2 is quite good. In case of Test 3, the values of the condition number $\kappa(\mathbf{A})$ are small, however, the max and RMS errors for certain values of γ are quite large. As we noted before, in comparison with first two examples, the problem of Test 3 demonstrates strong variability of the optimized values of the shape parameter ϵ respect to the values of γ (Table 4).

Table 6: Means and coefficients of variation of the optimized values of the MQ, IMQ, IQ and GA RBF shape parameter ϵ: γ was fixed ($\gamma = 1.0$), ξ or ξ_1 and ξ_2 were taken from random samples, $N = 100$.

		MQ	IMQ	IQ	GA
Problem with nonlocal condition (4a)					
Test 1					
Min. E_∞	Mean	0.546315913425	0.430805823852	0.37744328393	0.770526981203
	CV	0.0813345033203	0.0735449437812	0.0818600756345	0.0712298555533
Min. E_{RMS}	Mean	0.549479175927	0.431488028105	0.374954301061	0.747806248518
	CV	0.0779898974776	0.0743398400816	0.0803129755423	0.0647381252444
Test 2					
Min. E_∞	Mean	0.557503096986	0.516184931745	0.494956574381	1.21013053465
	CV	0.0770892746382	0.0517109472666	0.0464156197119	0.0199851228971
Min. E_{RMS}	Mean	0.558237874475	0.515593128694	0.495047086093	1.21249147426
	CV	0.0733901224165	0.0493699515919	0.0419489450382	0.0136891523163
Test 3					
Min. E_∞	Mean	0.87400434316	0.735345020775	0.629827256392	1.09668998936
	CV	0.203416588257	0.248985879667	0.323968263188	0.278191017196
Min. E_{RMS}	Mean	0.894950486667	0.711787791062	0.608660206287	1.04322442346
	CV	0.175515453781	0.278404586758	0.345538221098	0.262123943869
Problem with nonlocal condition (4b)					
Test 1					
Min. E_∞	Mean	0.547136960242	0.438461947242	0.37962472074	0.772480247923
	CV	0.0746507354983	0.0698962864618	0.0771201878261	0.0665456191321
Min. E_{RMS}	Mean	0.550950771558	0.437961637591	0.376241910714	0.749049259659
	CV	0.0727763106942	0.0662558304426	0.0761213209769	0.0637995571199
Test 2					
Min. E_∞	Mean	0.557234119818	0.516942330103	0.496838602999	1.20885970449
	CV	0.0804345786922	0.0528399287151	0.0444560188269	0.0236451902772
Min. E_{RMS}	Mean	0.559418143701	0.515536562689	0.496502902629	1.21242583379
	CV	0.0764892165455	0.0511041522461	0.0389659761057	0.0184332342373
Test 3					
Min. E_∞	Mean	0.877019139707	0.748647620942	0.645691834258	1.1364721472
	CV	0.198945039601	0.231401266138	0.30645410661	0.284531300503
Min. E_{RMS}	Mean	0.895240846084	0.721724355743	0.620950163321	1.06765376724
	CV	0.175135972162	0.26579208727	0.333327016418	0.272166898969

Table 7: Means and standard deviations of the optimized values of the GMQ RBF shape parameters β and ϵ: γ was fixed ($\gamma = 1.0$), ξ or ξ_1 and ξ_2 were taken from random samples, $N = 100$.

		β	ϵ
Problem with nonlocal boundary condition (4a)			
Test 1			
Min. E_∞	Mean	4.74456142802	0.624060484189
	SD	0.643796991784	0.199256856155
Min. E_{RMS}	Mean	4.84710145234	0.620347236419
	SD	0.685950413933	0.211737204314
Test 2			
Min. E_∞	Mean	−3.28316894379	0.744930098952
	SD	5.18752008151	0.648254143848
Min. E_{RMS}	Mean	−3.16305711488	0.749839271765
	SD	5.23217756706	0.637418004851
Test 3			
Min. E_∞	Mean	−6.13802710428	0.458521728453
	SD	2.92272727451	0.158001220648
Min. E_{RMS}	Mean	−5.67893121195	0.451279541776
	SD	3.67700265351	0.177729926948
Problem with nonlocal boundary condition (4b)			
Test 1			
Min. E_∞	Mean	4.70110441745	0.676268075106
	SD	0.631275189647	0.46894454569
Min. E_{RMS}	Mean	4.76018747229	0.651178575857
	SD	0.588448225975	0.369929183922
Test 2			
Min. E_∞	Mean	−2.50161509216	0.873165704983
	SD	5.626083594	0.718394281761
Min. E_{RMS}	Mean	−2.44591306921	0.865575438129
	SD	5.59699161737	0.702588376198
Test 3			
Min. E_∞	Mean	−6.13835049697	0.486864891083
	SD	2.70866487459	0.145758892753
Min. E_{RMS}	Mean	−5.7324111019	0.468138518305
	SD	3.50240080884	0.17492244483

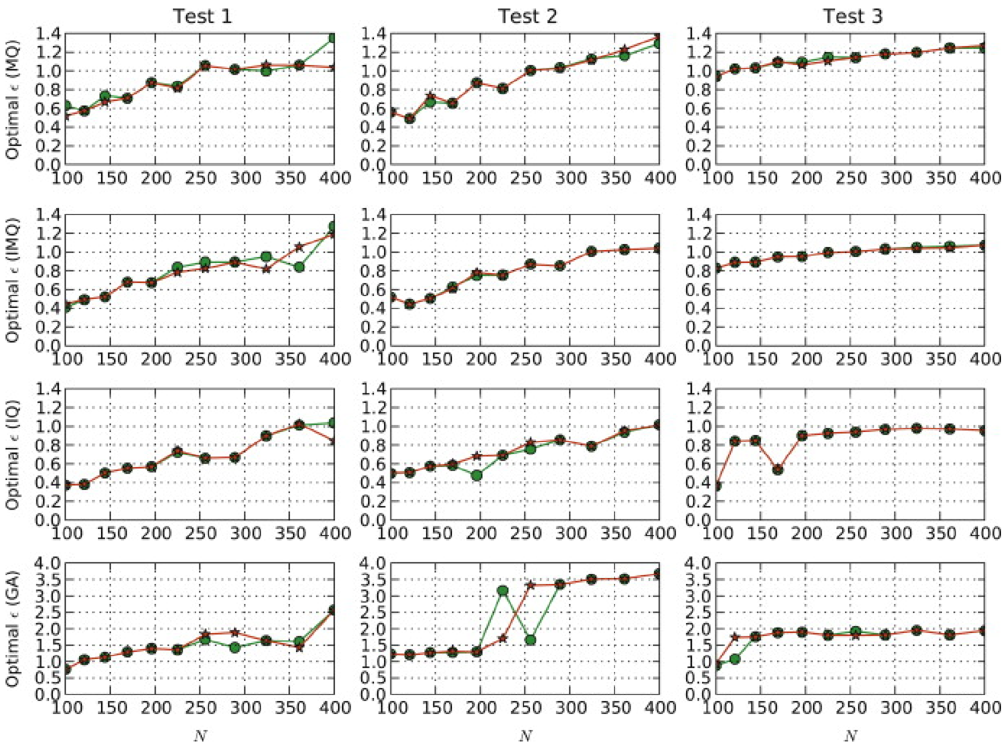

Figure 7: The dependence of the optimized values of the shape parameters on the number of centers N (centers are distributed uniformly): problem with nonlocal condition (4a), $\gamma = 1.0$, $\xi = 0.5$. The values of the shape parameter which minimize errors E_∞ and E_{RMS} are depicted as red curves with stars and green curves with bullets, respectively. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

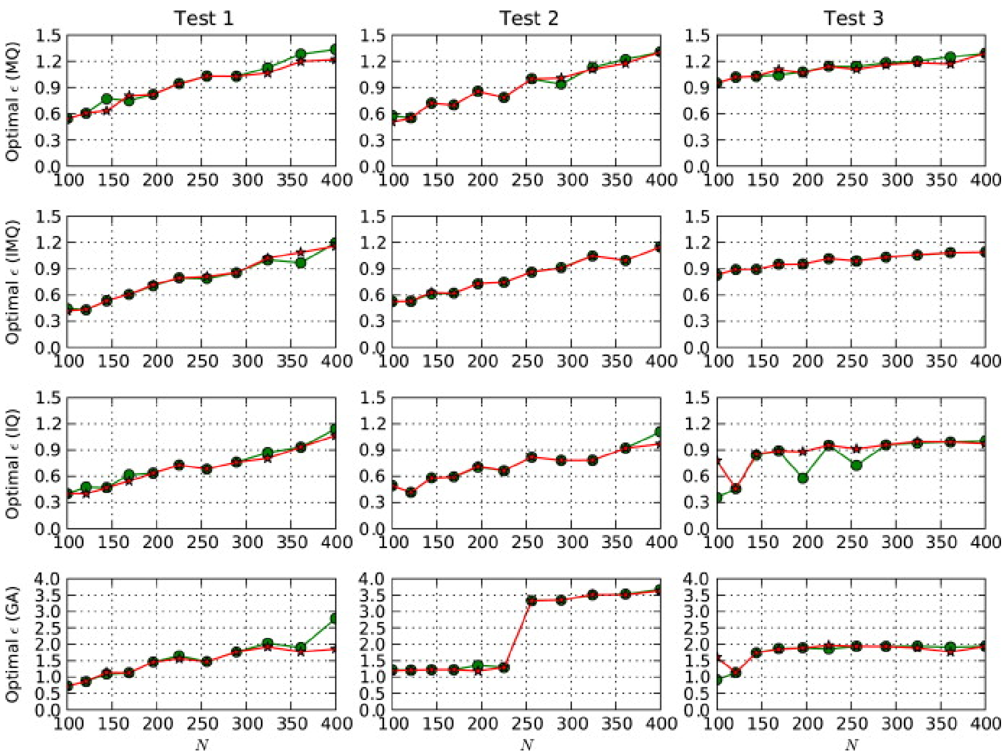

Figure 8: The dependence of the optimized values of the shape parameters on the number of centers N (centers are distributed uniformly): problem with nonlocal condition (4b), $\gamma = 1.0$, $\xi_1 = 0.0$, $\xi_2 = 1.0$. The values of the shape parameter which minimize errors E_∞ and E_{RMS} are depicted as red curves with stars and green curves with bullets, respectively. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

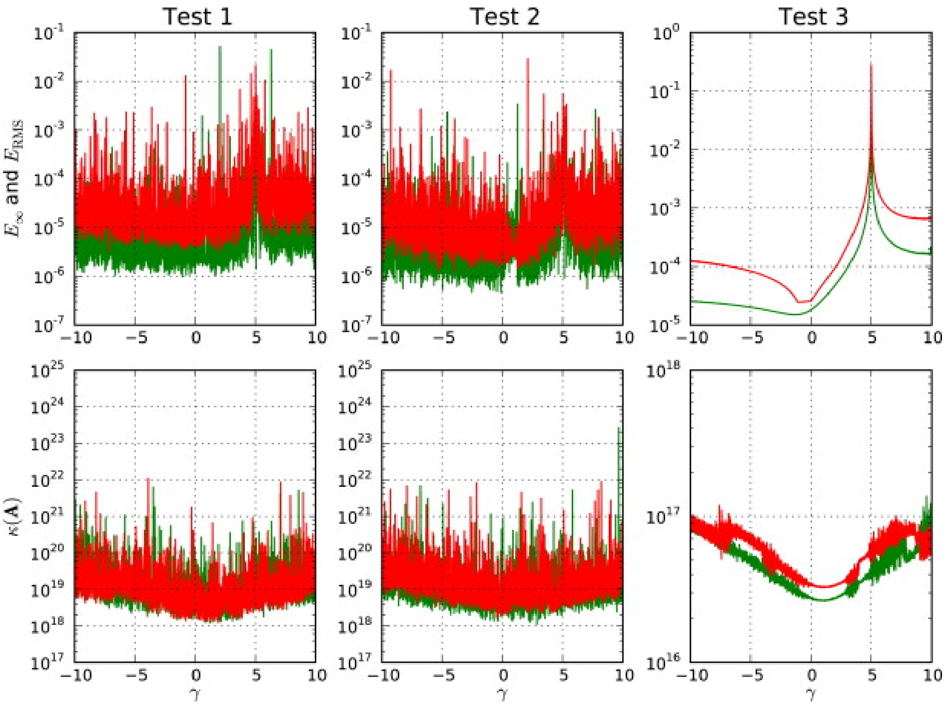

Figure 9: The dependence of the accuracy of the method and the condition number $\kappa(\mathbf{A})$ on the values of γ (red and green curves represent the data obtained using the values of the shape parameter ϵ minimizing errors E_∞ and $E_{\rm RMS}$, respectively): problem with nonlocal boundary condition (4a), $\xi = 0.5$; MQ RBF with the averaged optimized values of the shape parameter ϵ (Table 4) were used, $N = 100$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

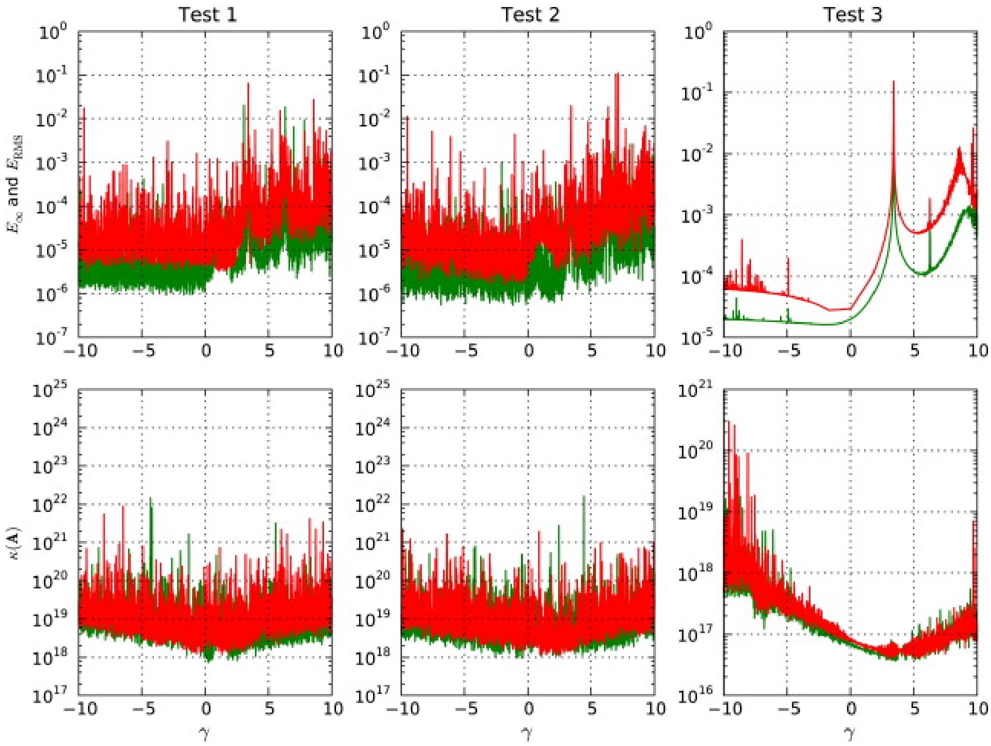

Figure 10: The dependence of the accuracy of the method and the condition number $\kappa(\mathbf{A})$ on the values of γ (red and green curves represent the data obtained using the values of the shape parameter ϵ minimizing errors E_∞ and $E_{\rm RMS}$, respectively): problem with nonlocal boundary condition (4b), $\xi_1 = 0.0$, $\xi_2 = 1.0$; MQ RBF with the averaged optimized values of the shape parameter ϵ (Table 4) were used, $N = 100$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

We also investigated how the conditioning and accuracy of the method depend on γ when the value of the shape parameter ϵ is fixed ($\epsilon = 1.0$). From the results obtained using MQ RBF and presented in Figs. 11 and 12 we see that the minimal values of the condition number $\kappa(\mathbf{A})$ arise with certain small positive values of γ. However, in general we note that when the value of $|\gamma|$ increases, the condition number also tends to increase.

In certain ranges of the values of γ, the spikes of the errors E_∞ and E_{RMS} are observable (see Figs. 11 and 12, and the results related with Test 3 in Figs. 9 and 10). From additional numerical experiments (the results are not presented here) we know that similar phenomena appear when other types of RBF are used (in case of GA RBF, the spikes are not very sharp). This issue needs further investigation.

The approximate solutions $\overline{u}(x, y)$ obtained using MQ, IMQ, IQ or GA RBF are accurate not only on the collocation points but also in the whole domain $[0, 1] \times [0, 1]$. In Figs. 13 and 14 we present the absolute errors $|u(x, y) - \overline{u}(x, y)|$, when approximate solutions $\overline{u}(x, y)$ of the problems are obtained using MQ, IMQ, IQ and GA RBF (the values of parameters in nonlocal conditions and the shape parameter ϵ are fixed).

From Figs. 15 and 16 we can see that when a total number of centers N grows, the accuracy of the method remains more or less stable (Test 1 and Test 2) or can be slightly increased (Test 3). The accuracy of the RBF technique can be increased significantly if extended precision floating point arithmetic is used for the computation [79].

4. Concluding remarks

The meshless method based on the RBF collocation technique for the solution of two-dimensional Poisson equation with nonlocal boundary condition was examined. We can formulate the following conclusions and remarks:

- As it is known, the conditioning and accuracy of the standard RBF-based meshless methods depends on the values of the RBF shape parameters (Figs. 3–6). In all the cases we analyzed, the variability of the optimized values of the shape parameter ϵ in MQ, IMQ, IQ and GA RBF respect to the values of γ or to the values of ξ or ξ_1 and ξ_2 is low (Tables 4 and 6). Discussed technique can give quite accurate results if averaged optimized values of the shape parameter are used (Figs. 9 and 10). More accurate results can be obtained if optimal or at least optimized (near-optimal) values of the shape parameter are used (Figs. 15 and 16). An efficient strategy for choosing optimal (near-optimal) value of the shape parameter would be very useful. Unfortunately, the optimal selection of the shape parameter depends on the problem and on the number of centers (Figs. 7 and 8). The closed-form approximate solution is accurate not only on the collocation points but also on the whole domain of the problem (Figs. 13 and 14).
- The variability of the optimized values of GMQ RBF parameters β and ϵ respect to the values of γ or to the values of ξ or ξ_1 and ξ_2 is high (Tables 5 and 7). In such cases, the accuracy of the results obtained using method with the averaged optimized values of the shape parameters can be poor. Therefore, while efficient strategy of the selection of the optimal values of the shape parameters is unknown, application of GMQ RBF for the numerical solution of similar differential problems can be complicated.
- In comparison with classical case ($\gamma = 0$), nonlocal boundary conditions can increase the condition number of the collocation matrix (Figs. 11 and 12). To avoid difficulties caused by this property of the method, a suitable stabilized linear solver or an efficient preconditioning technique can be used. This issue also seems to be sensitive to the precision of machine arithmetics.

It is important to note that these conclusions have been made from the results of numerical experiments with particular examples of the differential problem (1)–(4).

Numerical studies presented in the present and previous papers [48–51] demonstrate that the RBF-based meshless methods for the numerical solution of PDEs with nonlocal boundary conditions are promising. The RBF collocation technique can be successfully applied for the solution of the problems with various types of nonlocal boundary conditions. Moreover, this technique can be extended to multidimensional cases when the problems are formulated on irregularly shaped domains (for example of multidimensional steady-state differential problem with nonlocal boundary conditions see [80]). However, a lot of important practical and fundamental questions (such as the optimal selection of the shape parameters or the influence of nonlocal conditions on the invertibility of the collocation matrix) are still open. It is necessary to develop mathematical tools that are needed in order those questions to be answered.

The usage of the RBF-based meshless methods for time-dependent PDEs leads to additional interesting questions, for example, related with the time marching. The similar analysis of such methods for time-dependent PDEs with nonlocal boundary conditions also would be interesting.

Acknowledgment

The author is grateful to three anonymous reviewers for their constructive comments and suggestions which have improved the paper.

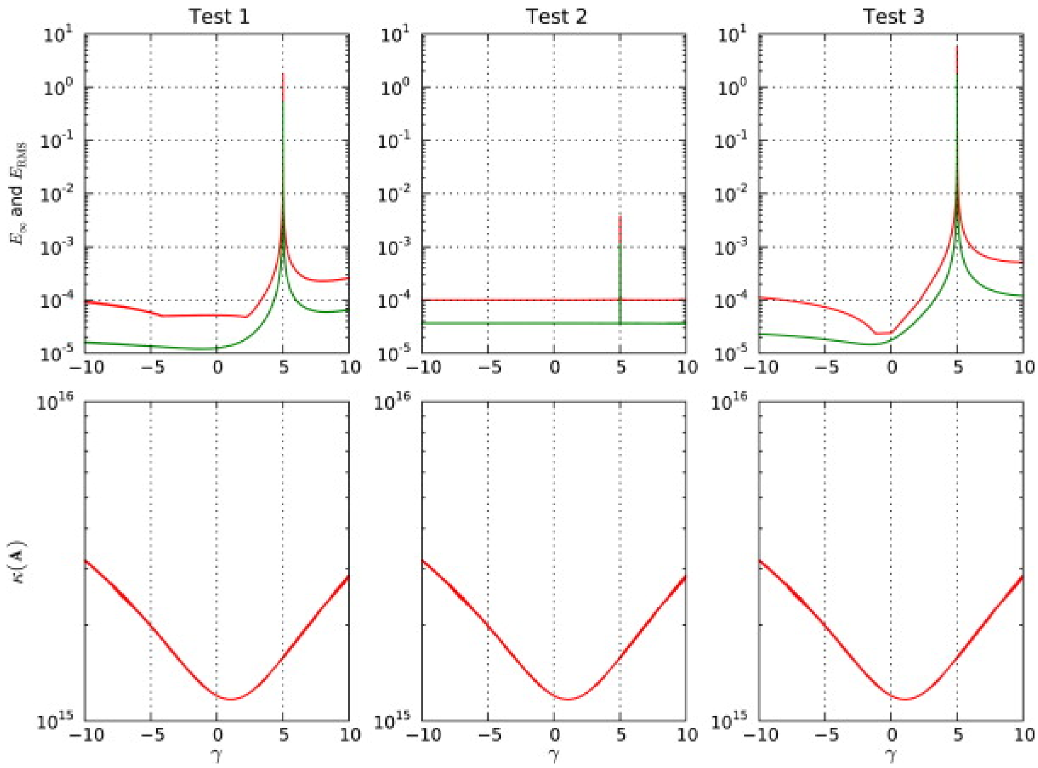

Figure 11: The dependence of the accuracy of the method (errors E_∞ and $E_{\rm RMS}$ are depicted as red curves and green curves, respectively) and the condition number $\kappa(\mathbf{A})$ (all three graphs in the second line represent the same data) on the values of γ: problem with nonlocal boundary condition (4a), $\xi = 0.5$; MQ RBF with $\epsilon = 1.0$ were used, $N = 100$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

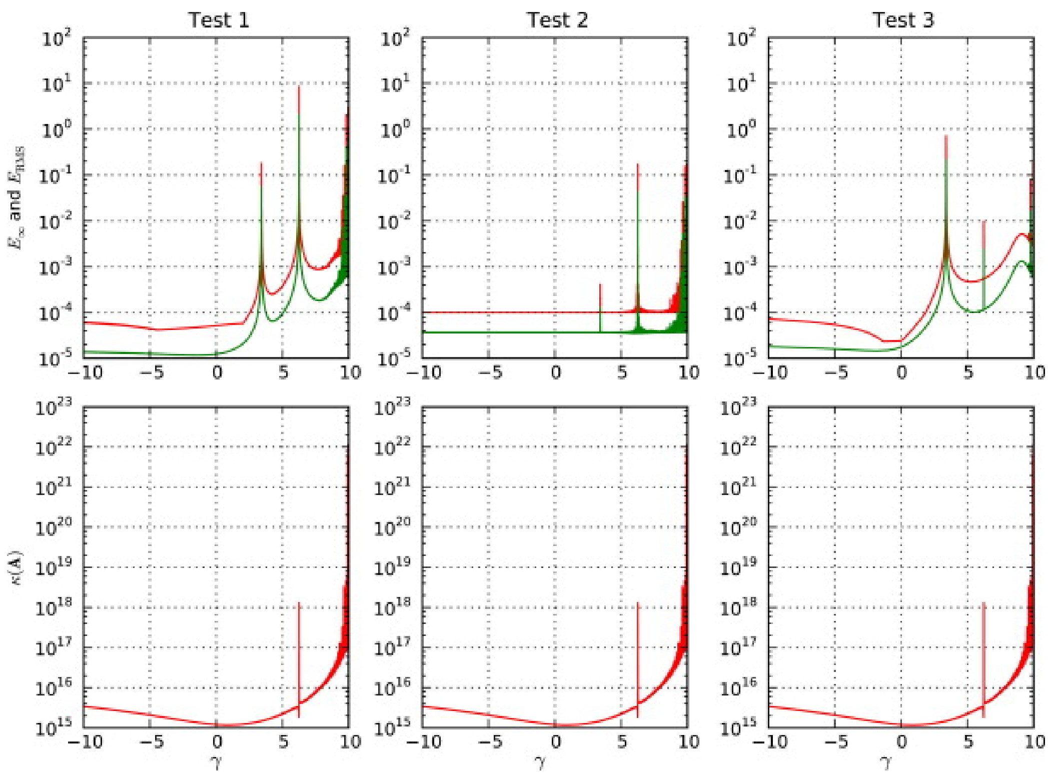

Figure 12: The dependence of the accuracy of the method (errors E_∞ and $E_{\rm RMS}$ are depicted as red curves and green curves, respectively) and the condition number $\kappa(\mathbf{A})$ (all three graphs in the second line represent the same data) on the values of γ: problem with nonlocal boundary condition (4b), $\xi_1 = 0.0$, $\xi_2 = 1.0$; MQ RBF with $\epsilon = 1.0$ were used, $N = 100$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

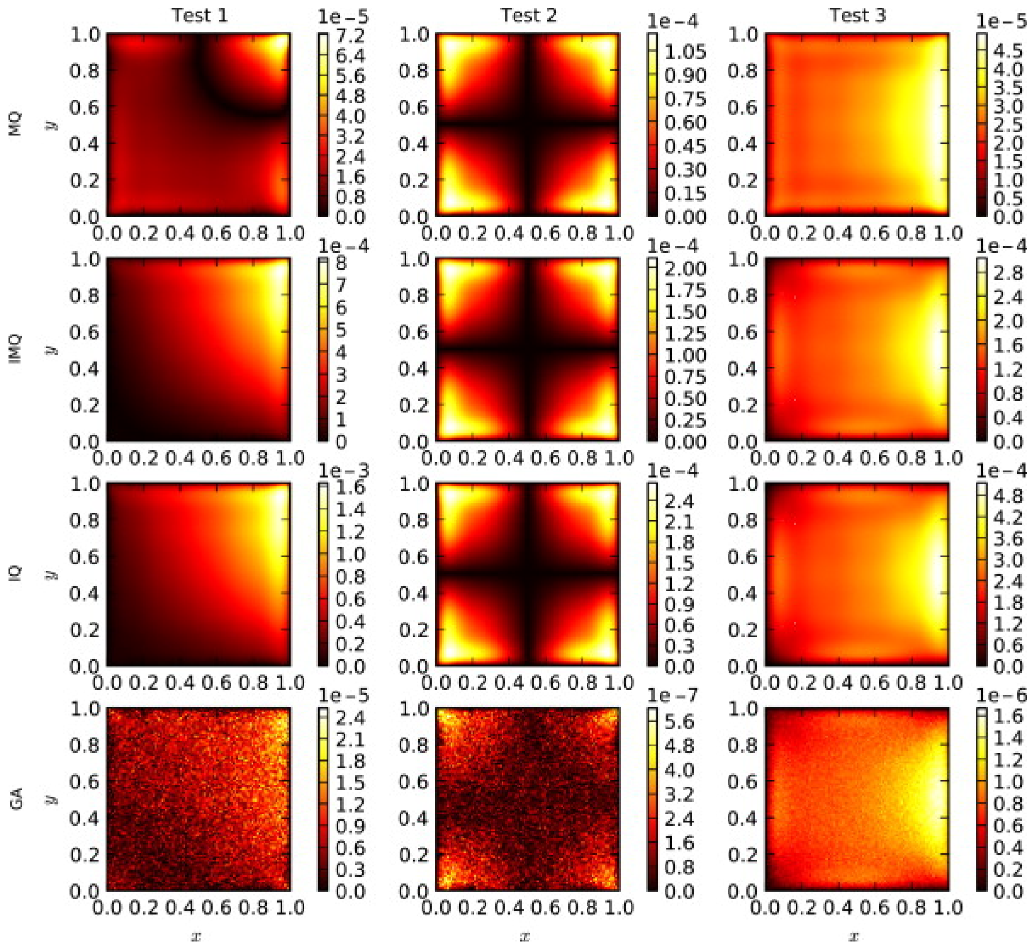

Figure 13: The absolute errors $|u(x, y) - \overline{u}(x, y)|$: problem with nonlocal boundary condition (4a), $\gamma = 1.0$, $\xi = 0.5$, $\epsilon = 1.0$, $N = 100$.

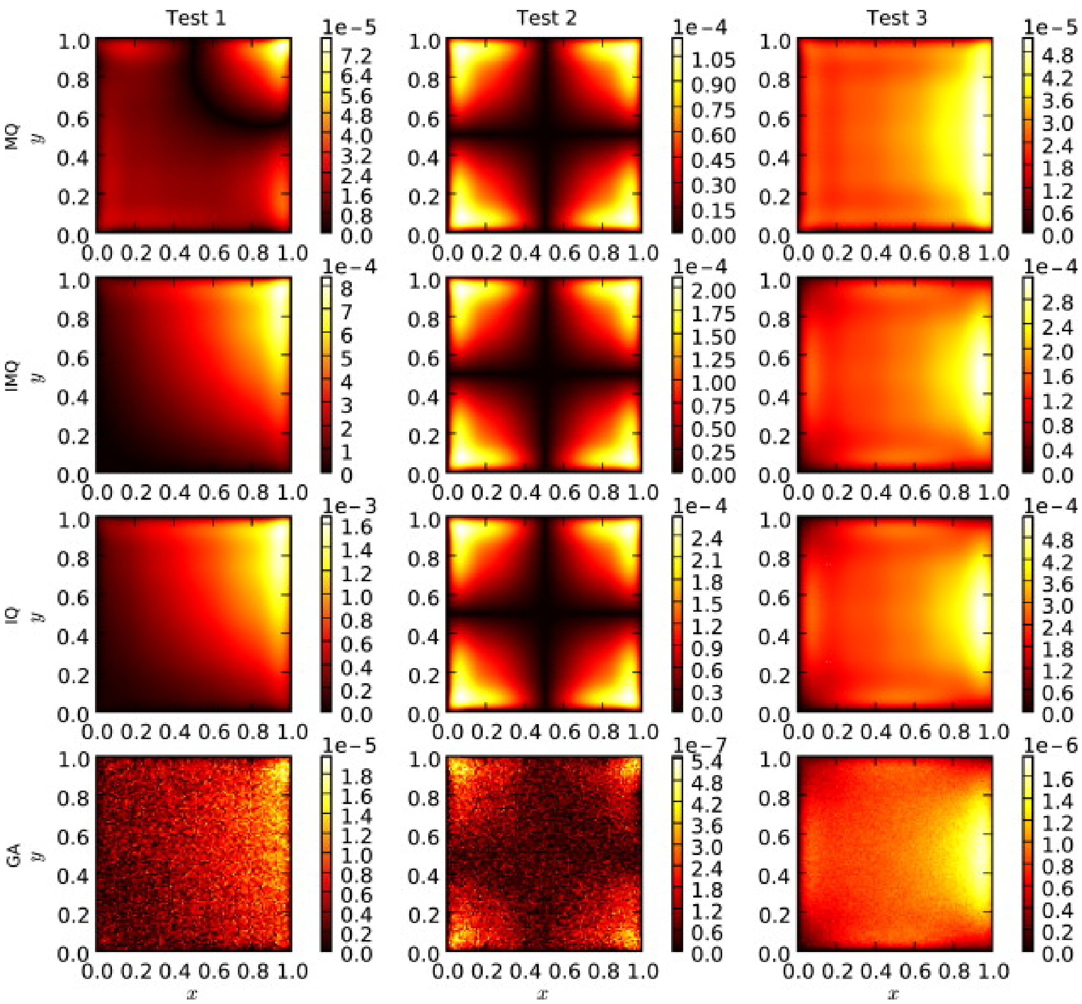

Figure 14: The absolute errors $|u(x, y) - \overline{u}(x, y)|$: problem with nonlocal boundary condition (4b), $\gamma = 1.0$, $\xi_1 = 0.0$, $\xi_2 = 1.0$, $\epsilon = 1.0$, $N = 100$.

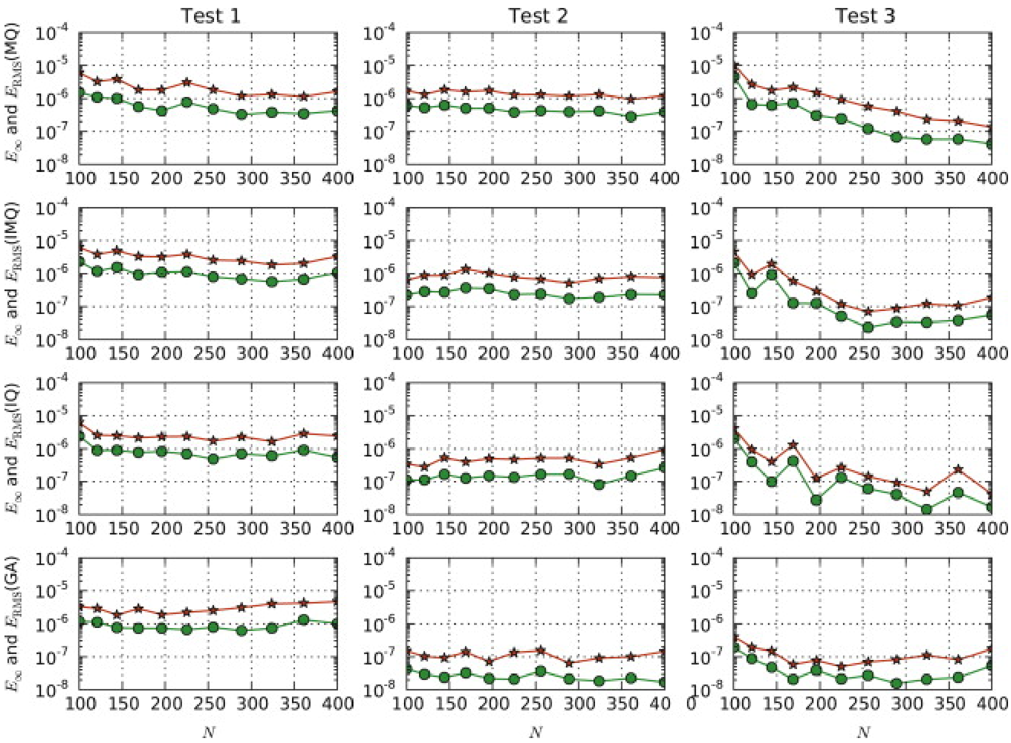

Figure 15: The dependence of the accuracy of the method (errors E_∞ and $E_{\rm RMS}$ are depicted as red curves with stars and green curves with bullets, respectively) on the number of centers N (centers are distributed uniformly): problem with nonlocal boundary condition (4a), $\gamma = 1.0$, $\xi = 0.5$; RBF with optimized values of the shape parameters (see Fig. 7) were used. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

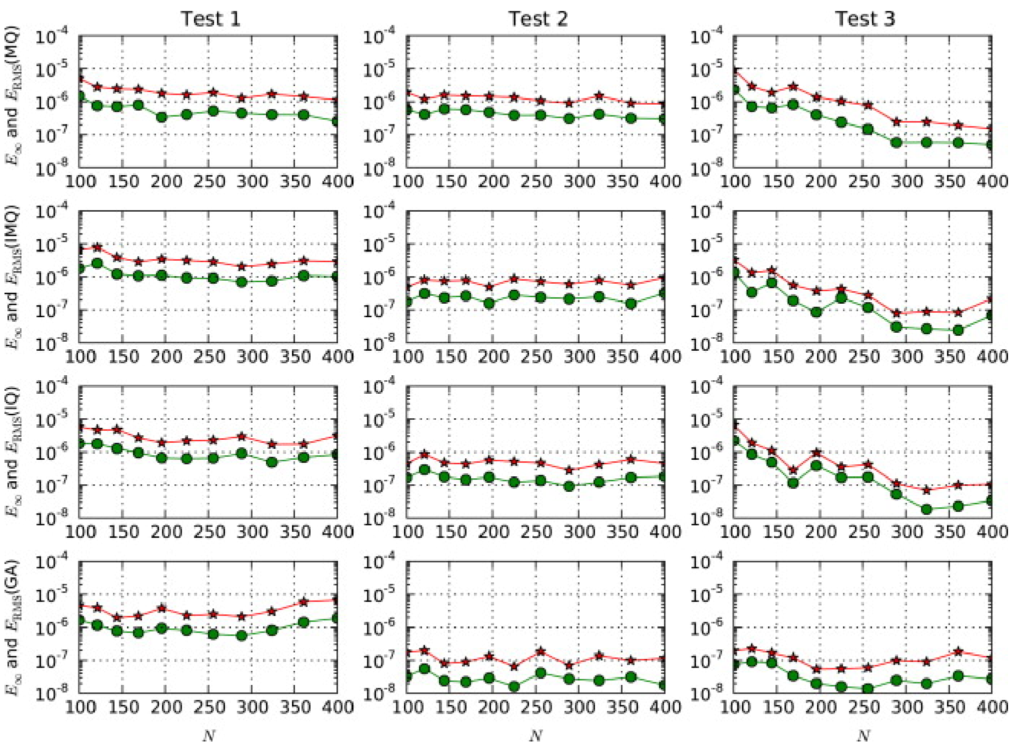

Figure 16: The dependence of the accuracy of the method (errors E_∞ and $E_{\rm RMS}$ are depicted as red curves with stars and green curves with bullets, respectively) on the number of centers N (centers are distributed uniformly): problem with nonlocal boundary condition (4b), $\gamma = 1.0$, $\xi_1 = 0.0$, $\xi_2 = 1.0$; RBF with optimized values of the shape parameters (see Fig. 8) were used. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

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