9 Boundary Value Problems: Collocation

We now present a different type of numerical method that will yield the approximate solution of a boundary value problem in the form of a function, as opposed to the set of discrete points resulting from the methods studied earlier. Just like the finite difference method, this method applies to both one-dimensional (two-point) boundary value problems, as well as to higher-dimensional elliptic problems (such as the Poisson problem).

We initially limit our discussion to the one-dimensional case. Assume we are given a general linear two-point boundary value problem of the form

$$\begin{aligned} Ly(t) &= f(t), \qquad t \in [a,b], \\ y(a) = \alpha&, \quad y(b) = \beta. \end{aligned} \tag{81}$$

To keep the discussion as general as possible, we now let

$$V = \operatorname{span}\{v_1, \ldots, v_n\}$$

denote an approximation space we wish to represent the approximate solution in. We can think of V as being, e.g., the space of polynomials or splines of a certain degree, or some *radial basis function space* (see more below).

We will express the approximate solution in the form

$$y(t) = \sum_{j=1}^{n} c_j v_j(t), \qquad t \in [a,b],$$

with unknown *coefficients* $c_1, \ldots, c_n$. Since L is assumed to be linear we have

$$Ly = \sum_{j=1}^{n} c_j L v_j,$$

and (81) becomes

$$\sum_{j=1}^{n} c_j L v_j(t) = f(t), \qquad t \in [a,b], \tag{82}$$

$$\sum_{j=1}^{n} c_j v_j(a) = \alpha, \quad \sum_{j=1}^{n} c_j v_j(b) = \beta.$$

In order to determine the n unknown coefficients $c_1, \ldots, c_n$ in this formulation we impose n *collocation conditions* to obtain an $n \times n$ system of linear equations for the c_j.

The last two equations in (82) ensure that the boundary conditions are satisfied, and give us the first two collocation equations. To obtain the other $n-2$ equations we choose $n-2$ *collocation points* $t_2, \ldots, t_{n-1}$, at which we enforce the differential equation. As in the previous numerical methods, this results in a discretization of the differential equation.

If we let $t_1 = a$ and $t_n = b$, then (82) becomes

$$\begin{aligned}
\sum_{j=1}^{n} c_j v_j(t_1) &= \alpha, \\
\sum_{j=1}^{n} c_j L v_j(t_i) &= f(t_i), \qquad i = 2, \ldots, n-1, \\
\sum_{j=1}^{n} c_j v_j(t_n) &= \beta.
\end{aligned}$$

In matrix form we have the linear system

$$\begin{bmatrix} v_1(t_1) & v_2(t_1) & \ldots & v_n(t_1) \\ Lv_1(t_2) & Lv_2(t_2) & \ldots & Lv_n(t_2) \\ \vdots & & & \vdots \\ Lv_1(t_{n-1}) & Lv_2(t_{n-1}) & \ldots & Lv_n(t_{n-1}) \\ v_1(t_n) & v_2(t_n) & \ldots & v_n(t_n) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} \alpha \\ f(t_2) \\ \vdots \\ f(t_{n-1}) \\ \beta \end{bmatrix}. \tag{83}$$

If the space V and the collocation points t_i, $i = 1, \ldots, n$, are chosen such that the collocation matrix in (83) is nonsingular then we can represent an approximate solution of (81) from the space V uniquely as

$$y(t) = \sum_{j=1}^{n} c_j v_j(t), \qquad t \in [a, b].$$

Remark Note that this provides the solution in the form of a function that can be evaluated anywhere in $[a, b]$. No additional interpolation is required as was the case with the earlier methods.

9.1 Radial Basis Functions for Collocation

The following discussion will apply to any sufficiently smooth admissible radial basic function. However, other basis functions such as polynomials or splines are also frequently used for collocation. In particular, the use of polynomials leads to so-called *spectral* or *pseudo-spectral* methods (see Chapter 11).

To initially keep our discussion as specific as possible we will choose the *multiquadric* basic function

$$\phi(r) = \sqrt{r^2 + \sigma^2}, \quad \sigma > 0,$$

with $r = |\cdot - t|$ the distance from a fixed center t. If we center one multiquadric at each of the collocation points t_j, $j = 1, \ldots, n$, then the approximation space becomes

$$V = \text{span}\{\phi(|\cdot - t_j|),\ j = 1, \ldots, n\}.$$

Now the system (83) becomes

$$\begin{bmatrix} \phi(|t_1-t_1|) & \phi(|t_1-t_2|) & \dots & \phi(|t_1-t_n|) \\ L\phi(|t_2-t_1|) & L\phi(|t_2-t_2|) & \dots & L\phi(|t_2-t_n|) \\ \vdots & & & \vdots \\ L\phi(|t_{n-1}-t_1|) & L\phi(|t_{n-1}-t_2|) & \dots & L\phi(|t_{n-1}-t_n|) \\ \phi(|t_n-t_1|) & \phi(|t_n-t_2|) & \dots & \phi(|t_n-t_n|) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} \alpha \\ f(t_2) \\ \vdots \\ f(t_{n-1}) \\ \beta \end{bmatrix}. \tag{84}$$

To get a better feel for this system we consider an example.

Example Let the differential operator L be given by

$$Ly(t) = y''(t) + wy'(t) + vy(t),$$

and ϕ denote the multiquadric radial basic function. Then

$$L\phi(|t-\tau|) = \phi''(|t-\tau|) + w\phi'(|t-\tau|) + v\phi(|t-\tau|)$$

with

$$\begin{aligned} \phi'(|t-\tau|) &= \frac{d}{dt}\phi(|t-\tau|) \\ &= \frac{d}{dt}\sqrt{|t-\tau|^2+\sigma^2} \\ &= \frac{t-\tau}{\sqrt{|t-\tau|^2+\sigma^2}} \end{aligned}$$

and

$$\begin{aligned} \phi''(|t-\tau|) &= \frac{d}{dt}\phi'(|t-\tau|) \\ &= \frac{d}{dt}\frac{t-\tau}{\sqrt{|t-\tau|^2+\sigma^2}} \\ &= \frac{\sqrt{|t-\tau|^2+\sigma^2} - \frac{(t-\tau)^2}{\sqrt{|t-\tau|^2+\sigma^2}}}{|t-\tau|^2+\sigma^2} \\ &= \frac{\sigma^2}{(|t-\tau|^2+\sigma^2)^{3/2}}. \end{aligned}$$

Therefore, we get

$$L\phi(|t-\tau|) = \frac{\sigma^2}{(|t-\tau|^2+\sigma^2)^{3/2}} + w\frac{t-\tau}{\sqrt{|t-\tau|^2+\sigma^2}} + v\sqrt{|t-\tau|^2+\sigma^2},$$

and the collocation matrix has entries of this type in rows 2 through $n-1$ with $\tau = t_j$, $j = 2, \dots, n-1$.

This method was suggested by Kansa (1990) and is one of the most popular approaches for solving boundary value problems with radial basis functions. The popularity of this method is due to the fact that it is simple to implement and it generalizes in a straightforward way to boundary value problems for elliptic partial differential equations in higher space dimensions.

For example, if we are given a domain $\Omega \subset \mathbb{R}^s$, and a linear elliptic partial differential equation of the form

$$Lu(\boldsymbol{x}) = f(\boldsymbol{x}), \qquad \boldsymbol{x} \text{ in } \Omega, \tag{85}$$

with, e.g., Dirichlet boundary conditions

$$u(\boldsymbol{x}) = g(\boldsymbol{x}), \qquad \boldsymbol{x} \text{ on } \partial\Omega. \tag{86}$$

Then, for Kansa's collocation method, we represent the approximate solution $\hat{u}$ by a radial basis function expansion of the form

$$\hat{u}(\boldsymbol{x}) = \sum_{j=1}^{N} c_j \phi(\|\boldsymbol{x} - \boldsymbol{\xi}_j\|). \tag{87}$$

As in the 1D-discussion above we formally distinguish in our notation between *centers* $\Xi = \{\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N\}$ and *collocation points* $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\} \subset \Omega$ even though these point sets will frequently coincide in practice. We will illustrate an example where $\Xi \neq \mathcal{X}$ at the end of this section. For the following discussion, however, we assume the simplest possible setting, i.e., , $\Xi = \mathcal{X}$.

The collocation matrix that arises when matching the differential equation (85) and the boundary conditions (86) at the collocation points $\mathcal{X}$ will be of the form

$$A = \begin{bmatrix} \tilde{A}_L \\ \tilde{A} \end{bmatrix}, \tag{88}$$

where the two blocks are generated as follows:

$$\begin{aligned} (\tilde{A}_L)_{ij} &= L\phi(\|\boldsymbol{x} - \boldsymbol{\xi}_j\|)|_{\boldsymbol{x}=\boldsymbol{x}_i}, \qquad \boldsymbol{x}_i \in \mathcal{I},\ \boldsymbol{\xi}_j \in \Xi, \\ \tilde{A}_{ij} &= \phi(\|\boldsymbol{x}_i - \boldsymbol{\xi}_j\|), \qquad \boldsymbol{x}_i \in \mathcal{B},\ \boldsymbol{\xi}_j \in \Xi. \end{aligned}$$

Here the set $\mathcal{X}$ of collocation points is split into a set $\mathcal{I}$ of interior points, and a set $\mathcal{B}$ of boundary points. The problem is well-posed if the linear system $A\boldsymbol{c} = \boldsymbol{y}$, with $\boldsymbol{y}$ a vector consisting of entries $f(\boldsymbol{x}_i)$, $\boldsymbol{x}_i \in \mathcal{I}$, followed by $g(\boldsymbol{x}_i)$, $\boldsymbol{x}_i \in \mathcal{B}$, has a unique solution.

We note that a change in the boundary conditions (86) is as simple as making changes to a few rows of the matrix A in (88) as well as on the right-hand side $\boldsymbol{y}$.

Remark 1. It was not known for a long time whether the matrix for this kind of radial basis function collocation was nonsingular for an arbitrary choice of basic function and arbitrary collocation points. However, recently Hon and Schaback (2001) showed that there exist configurations of collocation points (in the elliptic PDE setting in $\mathbb{R}^2$) for which the matrix will be singular for many of the most popular radial basic functions. On the other, while such configurations do exist they seem to be very rare.

2. This collocation method is closely related to a pseudospectral method (see Chapter 11) based on radial basis functions instead of polynomials.

It is obvious that the matrix in (84) or (88) is not symmetric. This means that many efficient linear algebra subroutines cannot be employed in its solution. Another approach to radial basis function collocation which yields a symmetric matrix was suggested by Fasshauer (1997).

We again begin our discussion of this method with the one-dimensional boundary value problem (81). However, now we use a different approximation space, namely

$$V = \mathrm{span}\{\phi(|\cdot - t_1|), \phi(|\cdot - t_n|)\} \cup \mathrm{span}\{L^{(2)}\phi(|\cdot - t_j|),\ j = 2, \ldots, n-1\}.$$

Here the operator $L^{(2)}$ is identical to L, but acts on ϕ as a function of the second variable t_j.

Since the approximate solution is now of the form

$$y(t) = c_1\phi(|t - t_1|) + \sum_{j=2}^{n-1} c_j L^{(2)}\phi(|t - t_j|) + c_n\phi(|t - t_n|) \tag{89}$$

we need to look at the collocation system one more time.

We start with (82), which — based on (89) — now becomes

$$\begin{aligned}
c_1\phi(|a - t_1|) + \sum_{j=2}^{n-1} c_j L^{(2)}\phi(|a - t_j|) + c_n\phi(|a - t_n|) &= \alpha, \\
c_1 L\phi(|t - t_1|) + \sum_{j=2}^{n-1} c_j LL^{(2)}\phi(|t - t_j|) + c_n L\phi(|t - t_n|) &= f(t), \qquad t \in [a, b], \\
c_1\phi(|b - t_1|) + \sum_{j=2}^{n-1} c_j L^{(2)}\phi(|b - t_j|) + c_n\phi(|b - t_n|) &= \beta.
\end{aligned}$$

If we enforce the collocation conditions at the interior points $t_2, \ldots, t_{n-1}$, then we get the system of linear equations

$$\begin{bmatrix}
\phi(|a - t_1|) & L^{(2)}\phi(|a - t_2|) & \ldots & L^{(2)}\phi(|a - t_{n-1}|) & \phi(|a - t_n|) \\
L\phi(|t_2 - t_1|) & LL^{(2)}\phi(|t_2 - t_2|) & \ldots & LL^{(2)}\phi(|t_2 - t_{n-1}|) & L\phi(|t_2 - t_n|) \\
\vdots & & & \vdots & \\
L\phi(|t_{n-1} - t_1|) & LL^{(2)}\phi(|t_{n-1} - t_2|) & \ldots & LL^{(2)}\phi(|t_{n-1} - t_{n-1}|) & L\phi(|t_{n-1} - t_n|) \\
\phi(|b - t_1|) & L^{(2)}\phi(|b - t_2|) & \ldots & L^{(2)}\phi(|b - t_{n-1}|) & \phi(|b - t_n|)
\end{bmatrix} \times$$

$$\times \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{n-1} \\ c_n \end{bmatrix} = \begin{bmatrix} \alpha \\ f(t_2) \\ \vdots \\ f(t_{n-1}) \\ \beta \end{bmatrix}. \tag{90}$$

Remark 1. The matrix in (90) is symmetric as claimed earlier. This is obvious if L is a differential operator of even order. For odd-order terms one can see that while differentiation with respect to the second variable introduces a sign change, this sign change is canceled by an interchange of the arguments so that $L\phi(|t_i - t_j|) = L^{(2)}\phi(|t_j - t_i|)$ (see the example below).

2. Depending on whether globally or locally supported radial basis functions are being used, we can now employ efficient linear solvers, such as Cholesky factorization or the conjugate gradient method, to solve this system.

3. The most important advantage of the symmetric collocation method over the non-symmetric one proposed by Kansa is that one can prove that the collocation matrix in the symmetric case is nonsingular for all of the standard radial basis functions and any choice of distinct collocation points.

4. Another benefit of using the symmetric form is that it is possible to give convergence order estimates for this case (see Theorem 9.1 below).

5. Since terms of the form $LL^{(2)}\phi$ are used, the symmetric collocation method has the disadvantage that it requires higher smoothness. Moreover, computing and coding these terms is more complicated than for the non-symmetric collocation method.

Example We again consider the differential operator L given by

$$Ly(t) = y''(t) + wy'(t) + vy(t),$$

and multiquadrics. Then

$$\begin{aligned} L^{(2)}\phi(|t-\tau|) &= \frac{d^2}{d\tau^2}\phi(|t-\tau|) + w\frac{d}{d\tau}\phi(|t-\tau|) + v\phi(|t-\tau|) \\ &= \frac{\sigma^2}{(|t-\tau|^2+\sigma^2)^{3/2}} - w\frac{t-\tau}{\sqrt{|t-\tau|^2+\sigma^2}} + v\sqrt{|t-\tau|^2+\sigma^2}, \end{aligned}$$

which is almost the same as $L\phi(|t-\tau|)$ in the earlier example except for the sign difference in the first derivative term. The higher-order terms are rather complicated. In the special case $w = v = 0$ we get

$$LL^{(2)}\phi(|t-\tau|) = \frac{15(t-\tau)^2\sigma^2}{(|t-\tau|^2+\sigma^2)^{7/2}} - \frac{3\sigma^2}{(|t-\tau|^2+\sigma^2)^{5/2}} + \frac{\sigma^2}{(|t-\tau|^2+\sigma^2)^{3/2}}.$$

In order to solve the higher-dimensional Dirichlet problem (85-86) with the symmetric collocation approach we use the expansion

$$\hat{u}(\boldsymbol{x}) = \sum_{j=1}^{N_{\mathcal{I}}} c_j L^{(2)}\varphi(\|\boldsymbol{x}-\boldsymbol{\xi}\|)|_{\boldsymbol{\xi}=\boldsymbol{\xi}_j} + \sum_{j=N_{\mathcal{I}}+1}^{N} c_j\varphi(\|\boldsymbol{x}-\boldsymbol{\xi}_j\|). \tag{91}$$

Here $N_{\mathcal{I}}$ denotes the number of nodes in the interior of Ω, and $L^{(2)}$ is the differential operator used in the differential equation (85), but acting on φ viewed as a function of the second argument, i.e., , $L\varphi$ is equal to $L^{(2)}\varphi$ up to a possible difference in sign.

After enforcing the collocation conditions

$$\begin{aligned} L\hat{u}(\boldsymbol{x}_i) &= f(\boldsymbol{x}_i), \qquad \boldsymbol{x}_i \in \mathcal{I}, \\ \hat{u}(\boldsymbol{x}_i) &= g(\boldsymbol{x}_i), \qquad \boldsymbol{x}_i \in \mathcal{B}, \end{aligned}$$

we end up with a collocation matrix A that is of the form

$$A = \begin{bmatrix} \hat{A}_{LL^{(2)}} & \hat{A}_L \\ \hat{A}_{L^{(2)}} & \hat{A} \end{bmatrix}. \tag{92}$$

Here the four blocks are generated as follows:

$$\begin{aligned}
(\hat{A}_{LL^{(2)}})_{ij} &= LL^{(2)}\varphi(\|\boldsymbol{x}-\boldsymbol{\xi}\|)|_{\boldsymbol{x}=\boldsymbol{x}_i,\boldsymbol{\xi}=\boldsymbol{\xi}_j}, \qquad \boldsymbol{x}_i,\boldsymbol{\xi}_j \in \mathcal{I}, \\
(\hat{A}_L)_{ij} &= L\varphi(\|\boldsymbol{x}-\boldsymbol{\xi}_j\|)|_{\boldsymbol{x}=\boldsymbol{x}_i}, \qquad \boldsymbol{x}_i \in \mathcal{I},\ \boldsymbol{\xi}_j \in \mathcal{B}, \\
(\hat{A}_{L^{(2)}})_{ij} &= L^{(2)}\varphi(\|\boldsymbol{x}_i-\boldsymbol{\xi}\|)|_{\boldsymbol{\xi}=\boldsymbol{\xi}_j}, \qquad \boldsymbol{x}_i, \in \mathcal{B},\ \boldsymbol{\xi}_j \in \mathcal{I}, \\
\hat{A}_{ij} &= \varphi(\|\boldsymbol{x}_i-\boldsymbol{\xi}_j\|), \qquad \boldsymbol{x}_i,\boldsymbol{\xi}_j \in \mathcal{B}.
\end{aligned}$$

Note that we have identified the two sets $\mathcal{X} = \mathcal{I} \cup \mathcal{B}$ of collocation points and Ξ of centers.

9.2 A Convergence Result

In the book "Scattered Data Approximation" by Holger Wendland one can find the following convergence result for the *symmetric* collocation method in arbitrarily many, s, space dimensions:

Theorem 9.1 *Let $\Omega \subseteq \mathbb{R}^s$ be a polygonal and open region. Let $L \neq 0$ be a second-order linear elliptic differential operator with coefficients in $C^{2(k-2)}(\bar{\Omega})$ that either vanish on $\bar{\Omega}$ or have no zero there. Suppose that $\Phi \in C^{2k}(\mathbb{R}^s)$ is a strictly positive definite function. Suppose further that the boundary value problem*

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

has a unique solution $u \in \mathcal{N}_\Phi(\Omega)$ for given $f \in C(\Omega)$ and $g \in C(\partial\Omega)$. Let $\hat{u}$ be the approximate collocation solution of the form

$$\hat{u}(\boldsymbol{x}) = \sum_{j=1}^{N_\mathcal{I}} c_j L^{(2)}\phi(\|\boldsymbol{x}-\boldsymbol{\xi}\|)|_{\boldsymbol{\xi}=\boldsymbol{\xi}_j} + \sum_{j=N_\mathcal{I}+1}^{N} c_j\phi(\|\boldsymbol{x}-\boldsymbol{\xi}_j\|).$$

based on $\Phi = \phi(\|\cdot\|)$. Then

$$\|u-\hat{u}\|_{L_\infty(\Omega)} \le Ch^{k-2}\|u\|_{\mathcal{N}_\Phi(\Omega)}$$

for all sufficiently small h, where h is the larger of the fill distances in the interior and on the boundary of Ω, respectively.

In order to understand this theorem we need to dig a little deeper into meshfree approximation methods. In particular, we need to understand the concepts of

- a *strictly positive definite function*,
- the *native space* $\mathcal{N}_\Phi(\Omega)$ of a given strictly positive definite function Φ, and

- the *fill distance* of a set of points in $\mathbb{R}^s$.

Definition 9.2 *A real-valued continuous function Φ is positive definite on $\mathbb{R}^s$ if and only if it is even and*

$$\sum_{j=1}^{N}\sum_{k=1}^{N} c_j c_k \Phi(\boldsymbol{x}_j - \boldsymbol{x}_k) \geq 0 \tag{93}$$

for any N pairwise different points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^s$, and $\boldsymbol{c} = [c_1, \ldots, c_N]^T \in \mathbb{R}^N$.

The function Φ is strictly positive definite on $\mathbb{R}^s$ if the quadratic form (93) is zero only for $\boldsymbol{c} \equiv \boldsymbol{0}$.

In order to introduce the concept of the native space of a strictly positive definite function we actually consider strictly positive definite *kernels* K which we can think of begin connected to the radial basic function ϕ by $K(\boldsymbol{x}, \boldsymbol{y}) = \Phi(\boldsymbol{x} - \boldsymbol{y}) = \phi(\|\boldsymbol{x} - \boldsymbol{y}\|)$. Native spaces are in fact reproducing kernel Hilbert spaces $\mathcal{H}$, i.e., real Hilbert function spaces with a *reproducing kernel* $K : \Omega \times \Omega \to \mathbb{R}$ and inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. In particular, the reproducing kernel K satisfies

1. $K(\cdot, \boldsymbol{x}) \in \mathcal{H}$ for all $\boldsymbol{x} \in \Omega$,
2. $f(\boldsymbol{x}) = \langle f, K(\cdot, \boldsymbol{x}) \rangle_{\mathcal{H}}$ for all $f \in \mathcal{H}$ and all $\boldsymbol{x} \in \Omega$.

It is this second *reproducing property* that inspires the name *reproducing kernel*.

In order to understand the native space of a strictly positive definite function $\Phi(\cdot - \cdot) = K(\cdot, \cdot)$ we now consider the space $H_K(\Omega)$ of all functions f of the form

$$f = \sum_{j=1}^{N_K} c_j K(\cdot, \boldsymbol{x}_j)$$

provided $\boldsymbol{x}_j \in \Omega$. Here $N_K = \infty$ is allowed. Next we define a bilinear form $\langle \cdot, \cdot \rangle_K$ by

$$\langle f, g \rangle_K = \langle \sum_{j=1}^{N_K} c_j K(\cdot, \boldsymbol{x}_j), \sum_{k=1}^{N_K} d_k K(\cdot, \boldsymbol{y}_k) \rangle_K = \sum_{j=1}^{N_K}\sum_{k=1}^{N_K} c_j d_k K(\boldsymbol{x}_j, \boldsymbol{y}_k).$$

which induces a norm $\|f\|_K^2 = \langle f, f \rangle_K$. One can then show

Theorem 9.3 *If $K : \Omega \times \Omega \to \mathbb{R}$ is a symmetric strictly positive definite kernel, then the bilinear form $\langle \cdot, \cdot \rangle_K$ defines an inner product on $H_K(\Omega)$. Furthermore, $H_K(\Omega)$ is a pre-Hilbert space with reproducing kernel K.*

Furthermore, since we just established that $H_K(\Omega)$ is a pre-Hilbert space, i.e., , need not be complete, we now define the *native space* $\mathcal{N}_K(\Omega)$ of K to be the completion of $H_K(\Omega)$ with respect to the K-norm $\|\cdot\|_K$ so that $\|f\|_K = \|f\|_{\mathcal{N}_K(\Omega)}$ for all $f \in H_K(\Omega)$. The details of this construction are too involved to be discussed here.

It turns out that some radial basic functions have very "natural" native spaces, while the native space for other radial basic functions is rather small.

Example 1. Multiquadrics $\phi(r) = \sqrt{r^2 + \sigma^2}$, inverse multiquadrics $\phi(r) = 1/sqrtr^2 + \sigma^2$ and Gaussians $\phi(r) = e^{-\sigma^2 r^2}$ have very small native spaces.

2. Matérn functions or Sobolev splines $\phi(r) = \frac{K_{\beta-\frac{s}{2}}(r)r^{\beta-\frac{s}{2}}}{2^{\beta-1}\Gamma(\beta)}$, $\beta > \frac{s}{2}$ have Sobolev spaces as their native spaces. Here K_ν is the *modified Bessel function of the second kind*.

3. Polyharmonic splines $\phi(r) = r^\beta$, $0 < \beta \notin 2\mathbb{N}$ or $\phi(r) = r^{2\beta}\log r$, $\beta \in \mathbb{N}$ have so-called Beppo-Levi spaces (or homogeneous Sobolev spaces) as their native spaces.

One uses the fill distance as a one way to measure the data distribution in higher-dimensional spaces. The fill distance is usually defined as

$$h = h_{\mathcal{X},\Omega} = \sup_{\boldsymbol{x}\in\Omega} \min_{\boldsymbol{x}_j\in\mathcal{X}} \|\boldsymbol{x} - \boldsymbol{x}_j\|_2, \tag{94}$$

and it indicates how well the data in the set $\mathcal{X}$ fill out the domain Ω. A geometric interpretation of the fill distance is given by the radius of the largest possible empty ball that can be placed among the data locations inside Ω (see Figure 7 for a 2D illustration). Sometimes the synonym *covering radius*is used. Figure 7 illustrates the fill distance for a set of 25 Halton points. Note that in this case the largest "hole" in the data is near the boundary.

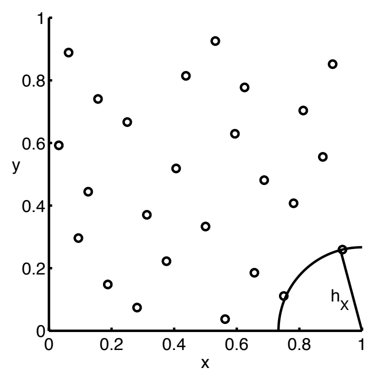

Figure 7: The fill distance for $N = 25$ Halton points ($h_{\mathcal{X},\Omega} \approx 0.2667$).

As a consequence of the proof of the convergence theorem (Theorem 9.1) Wendland suggests that the collocation points and centers be chosen so that the fill distance on the boundary is smaller than in the interior since the approximation orders differ by a factor ℓ (for differential operators of order ℓ). More precisely, he suggests distributing the points so that

$$h_{\mathcal{I},\Omega}^{k-\ell} \approx h_{\mathcal{B},\partial\Omega}^{k}.$$

More on radial basis function collocation methods is discussed in my book "Meshfree Approximation Methods with MATLAB".

Some numerical evidence for convergence rates of the symmetric collocation method is given by the following two-dimensional examples.

Example In the MATLAB script `KansaLaplace_2D.m` we solve the PDE

$$\begin{aligned}
\nabla^2 u(x,y) &= -\frac{5}{4}\pi^2 \sin(\pi x)\cos\left(\frac{\pi y}{2}\right), \quad (x,y) \in \Omega = [0,1]^2, \\
u(x,y) &= \sin(\pi x), \quad (x,y) \in \Gamma_1, \\
u(x,y) &= 0, \quad (x,y) \in \Gamma_2,
\end{aligned}$$

where $\Gamma_1 = \{(x,y): \ 0 \le x \le 1, \ y = 0\}$ and $\Gamma_2 = \partial\Omega \setminus \Gamma_1$. As can easily be verified, the exact solution is given by

$$u(x,y) = \sin(\pi x)\cos\left(\frac{\pi y}{2}\right).$$

In Tables 6 and 7 we list RMS-errors and condition numbers for the non-symmetric collocation solution of the PDE problem above. In Table 6 and the right part of Table 7 we present results for collocation with inverse multiquadric RBFs using a shape parameter of $\sigma = 3$, $N = 289$ interior, and an additional 64 boundary collocation points. In Table 6 the interior points are irregularly spaced Halton points, while in Table 7 we use uniformly spaced interior points. The boundary centers are placed outside the domain for the results in Table 7. In Table 6 we compare the effect of placing the boundary centers directly on the boundary (coincident with the boundary collocation points) as opposed to placement outside the domain.

N	centers on boundary		centers outside	
(interior points)	RMS-error	cond(A)	RMS-error	cond(A)
9	5.642192e-002	5.276474e+002	6.029293e-002	4.399608e+002
25	1.039322e-002	3.418858e+003	4.187975e-003	2.259698e+003
81	2.386062e-003	1.726995e+006	4.895870e-004	3.650369e+005
289	4.904715e-005	1.706884e+010	2.668524e-005	5.328110e+009
1089	3.676576e-008	1.446865e+018	1.946954e-008	5.015917e+017

Table 6: Non-symmetric collocation solution with IMQs, $\sigma = 3$ and interior Halton points.

The left part of Table 7 compares the use of Gaussians (with the same shape parameter $\sigma = 3$) to inverse multiquadrics.

Several observations can be made by looking at Tables 6 and 7. The use of Halton points instead of uniform points seems to be beneficial since both the errors and the condition numbers are smaller (cf. the right part of Table 6 vs. the right part of Table 7). Placement of the boundary centers outside the domain seems to be advantageous since again both the errors and the condition numbers decrease (cf. Table 6). Also, the last row of Table 7 seems to indicate that Gaussians are more prone to ill-conditioning than inverse multiquadrics.

Of course, these are rather superficial observations based on only a few numerical experiments. For many of these claims there is no theoretical foundation, and many more experiments would be needed to make a more conclusive statement (for example,

N	Gaussian		IMQ	
(interior points)	RMS-error	cond(A)	RMS-error	cond(A)
3×3	1.981675e-001	1.258837e+003	1.526456e-001	2.794516e+002
5×5	7.199931e-003	4.136193e+003	6.096534e-003	2.409431e+003
9×9	1.947108e-004	2.529708e+010	8.071271e-004	8.771630e+005
17×17	4.174290e-008	5.335000e+019	3.219110e-005	5.981238e+010
33×33	1.408750e-005	7.106505e+020	1.552047e-007	1.706638e+020

Table 7: Non-symmetric collocation solution with Gaussians and IMQs, $\sigma = 3$ and uniform interior points and boundary centers outside the domain.

no attempt was made here to find the best approximations, i.e., , optimize the value of the shape parameter). Also, one could experiment with different values of the shape parameter on the boundary and in the interior.

Example The problem dealt with in the second script `KansaLaplaceMixedBC_2D.m` is

$$\begin{aligned}
\nabla^2 u(x,y) &= -5.4x, \quad (x,y) \in \Omega = [0,1]^2, \\
\frac{\partial}{\partial \boldsymbol{n}} u(x,y) &= 0, \quad (x,y) \in \Gamma_1 \cup \Gamma_3, \\
u(x,y) &= 0.1, \quad (x,y) \in \Gamma_2, \\
u(x,y) &= 1, \quad (x,y) \in \Gamma_4,
\end{aligned}$$

where

$$\begin{aligned}
\Gamma_1 &= \{(x,y): \ 0 \le x \le 1, \ y = 0\}, \\
\Gamma_2 &= \{(x,y): \ x = 1, \ 0 \le y \le 1\}, \\
\Gamma_3 &= \{(x,y): \ 0 \le x \le 1, \ y = 1\}, \\
\Gamma_4 &= \{(x,y): \ x = 0, \ 0 \le y \le 1\}.
\end{aligned}$$

For this problem the exact solution is given by

$$u(x,y) = 1 - 0.9x^3.$$

In Table 8 we again compare the use of Gaussians and inverse multiquadrics on a set of $N = 9, 25, 81, 289$ and 1089 interior Halton points (with additional boundary centers outside the domain). As in the previous experiments the Gaussian solution is slightly inferior in terms of stability for the same value of the shape parameter.

In the following two examples we illustrate the use of the symmetric collocation method. The implementation is more complicated since we now also need fourth-order derivatives of the basic function, i.e., for the Laplace problems discussed above we now

N	Gaussian		IMQ	
(interior points)	RMS-error	cond(A)	RMS-error	cond(A)
9	3.423330e-001	5.430073e+003	7.937403e-002	2.782348e+002
25	1.065826e-002	1.605086e+003	5.605445e-003	1.680888e+003
81	5.382387e-004	3.684159e+008	1.487160e-003	2.611650e+005
289	6.181855e-006	1.452124e+019	1.822077e-004	3.775455e+009
1089	2.060470e-006	1.628262e+021	1.822221e-007	3.155751e+017

Table 8: Non-symmetric collocation solution with Gaussians and IMQs, $\sigma = 3$ and interior Halton points.

require also the differential operator

$$\begin{aligned}\nabla^2_{(2)}\nabla^2 &= \left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right)\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\\ &= \left(\frac{\partial^2}{\partial\xi^2}\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial\eta^2}\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial\xi^2}\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial\eta^2}\frac{\partial^2}{\partial y^2}\right)\\ &= \left(\frac{\partial^4}{\partial x^4}+2\frac{\partial^4}{\partial x^2 y^2}+\frac{\partial^4}{\partial y^4}\right),\end{aligned}$$

where the simplification in the last line is justified since we are working with even-order derivatives. For example, using the chain rule with $r = \|\boldsymbol{x}-\boldsymbol{\xi}\|$ we get for various radial basis functions in $\mathbb{R}^2$:

$$\begin{aligned}\nabla^2_{(2)}\nabla^2 e^{-(\sigma r)^2} &= 16\sigma^4\left(2-4(\sigma r)^2+(\sigma r)^4\right)e^{-(\sigma r)^2}, \text{ Gaussian}\\ \nabla^2_{(2)}\nabla^2\frac{1}{\sqrt{1+(\sigma r)^2}} &= \frac{3\sigma^4\left(3(\sigma r)^4-24(\sigma r)^2+8\right)}{\left(1+(\sigma r)^2\right)^{9/2}}, \quad \text{IMQ},\\ \nabla^2_{(2)}\nabla^2\sqrt{1+(\sigma r)^2} &= \frac{\sigma^4\left((\sigma r)^4+8(\sigma r)^2-8\right)}{\left(1+(\sigma r)^2\right)^{7/2}}, \quad \text{MQ}.\end{aligned}$$

Example In the MATLAB script `HermiteLaplace_2D.m` we solve the same problem as in `KansaLaplace_2D.m`. The same set of experiments as for the non-symmetric Kansa method (see Tables 6 and 7) are displayed in Tables 9 and 10 for the symmetric Hermite-based method.

We note that, as for the non-symmetric collocation method, inverse multiquadrics with interior Halton points and exterior boundary centers seems to perform overall slightly better than the other choices (i.e., , Gaussians, interior uniform points, or boundary centers on the boundary).

It is remarkable how small the difference in performance between the symmetric and non-symmetric approach is.

This example shows very high convergence rates as predicted by the estimate in Theorem 9.1 when using infinitely smooth inverse multiquadrics on a problem that has a smooth solution.

N	centers on boundary		centers outside	
(interior points)	RMS-error	cond(A)	RMS-error	cond(A)
9	1.869505e-001	9.055720e+003	2.438041e-001	3.549895e+004
25	7.698471e-002	8.506782e+004	9.429580e-002	1.162027e+005
81	4.839682e-003	1.338599e+007	5.070833e-003	1.017388e+007
289	4.480250e-005	9.991615e+010	3.448546e-005	7.180249e+010
1089	2.481407e-008	2.820823e+018	1.907000e-008	2.262777e+018

Table 9: Symmetric collocation solution with IMQs, $\sigma = 3$ and Halton points.

N	Gaussian		IMQ	
(interior points)	RMS-error	cond(A)	RMS-error	cond(A)
3×3	4.088188e-001	1.196486e+005	2.806897e-001	3.105155e+004
5×5	7.704584e-003	1.359899e+005	1.583948e-001	1.216534e+005
9×9	2.272289e-004	2.453107e+010	8.650782e-004	2.016503e+007
17×17	5.271776e-008	4.338406e+021	3.962654e-005	6.051588e+011
33×33	5.805757e-007	1.438258e+022	1.870210e-007	2.324115e+020

Table 10: Symmetric collocation solution with Gaussians and IMQs, $\varepsilon = 3$ and uniform points with boundary centers outside the domain.

Example Instead of repeating the calculations for Example **??**, we present a different problem with piecewise defined boundary conditions.

$$
\begin{aligned}
\nabla^2 u(x,y) &= 0, \quad (x,y) \in \Omega = (-1,1)^2, \\
u(x,y) &= 0, \quad (x,y) \in \Gamma_1 \cup \Gamma_3 \cup \Gamma_5, \\
u(x,y) &= \frac{1}{5}\sin(3\pi y), \quad (x,y) \in \Gamma_2, \\
u(x,y) &= \sin^4(\pi x), \quad (x,y) \in \Gamma_4,
\end{aligned}
$$

where

$$
\begin{aligned}
\Gamma_1 &= \{(x,y):\ -1 \le x \le 1,\ y = -1\}, \\
\Gamma_2 &= \{(x,y):\ x = 1,\ -1 \le y \le 1\}, \\
\Gamma_3 &= \{(x,y):\ 0 \le x \le 1,\ y = 1\}, \\
\Gamma_4 &= \{(x,y):\ -1 \le x \le 0,\ y = 1\}, \\
\Gamma_5 &= \{(x,y):\ x = -1,\ 0 \le y \le 1\}.
\end{aligned}
$$

For this problem we do not have an exact solution available. However, this problem is taken from [**?**] and we use the pseudospectral solution from there for comparison. We will revisit this problem later when we discuss RBF-PS methods in Chapter **??**.

The definition of the boundary conditions in the MATLAB code for `HermiteLaplaceMixedBCTref_2D.m` is similar to that for `KansaLaplaceMixedBC_2D.m`. However, now we are working on the square $[-1, 1]^2$ instead of $[0, 1]^2$, and therefore slight adjustments are required. For example, the collocation points have to be transformed, and the boundary centers have to be offset from a different boundary.

9.3 Summarizing Remarks on the Symmetric and Non-Symmetric RBF Collocation Methods

All in all, the non-symmetric (Kansa) method seems to perform just a little bit better than the symmetric (Hermite) method (compare Tables 6 and 7 with Tables 9 and 10). For the same value of the shape parameter σ the errors as well as the condition numbers are slightly smaller.

An advantage of the Hermite approach over Kansa's method is that the collocation matrices resulting from the Hermite approach are symmetric if all of the centers coincide with the collocation points. Therefore the amount of computation can be reduced considerably by using a solver for symmetric systems. Since Kansa's method requires fewer derivatives of the basic function it has the added advantages of being simpler to implement and applicable to problems with less smooth solutions. Moreover, the non-symmetric method is much simpler for problems with non-constant coefficients. Furthermore, it is not clear how to deal with non-linear problems using the symmetric method.

Another contraposition of the two methods appears in the context of pseudospectral methods which we will discuss in a later chapter.