Meshless algorithm for partial differential equations on open and singular surfaces

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Meshless Algorithm for Partial Differential Equations on Open and Singular Surfaces

CHEUNG Ka Chun

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy

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March 2016
Declaration

I hereby declare that this thesis represents my own work which has been done after registration for the degree of PhD at Hong Kong Baptist University, and has not been previously included in a thesis or dissertation submitted to this or any other institution for a degree, diploma or other qualifications.

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Abstract

Radial Basis function (RBF) method for solving partial differential equation (PDE) has a lot of applications in many areas. One of the advantages of RBF method is meshless. The cost of mesh generation can be reduced by playing with scattered data. It can also allow adaptivity to solve some problems with special feature. In this thesis, RBF method will be considered to solve several problems. Firstly, we solve the PDEs on surface with singularity (folded surface) by a localized method. The localized method is a generalization of finite difference method. A priori error estimate for the discretization of Laplace operator is given for points selection. A stable solver (RBF-QR) is used to avoid ill-conditioning for the numerical simulation.

Secondly, a $H^2$ convergence study for the least-squares kernel collocation method, a.k.a. least-square Kansa’s method will be discussed. This chapter can be separated into two main parts: constraint least-square method and weighted least-square method. For both methods, stability and consistency analysis are considered. Error estimate for both methods are also provided. For the case of weighted least-square Kansa’s method, we figured out a suitable weighting for optimal error estimation.

In Chapter two, we solve partial differential equation on smooth surface by an embedding method in the embedding space $\mathbb{R}^d$. Therefore, one can apply any numerical method in $\mathbb{R}^d$ to solve the embedding problem. Thus, as an application of previous result, we solve embedding problem by least-squares kernel collocation. Moreover, we propose a new embedding condition in this chapter which has high order of convergence. As a result, we solve partial differential equation on smooth surface with a high order kernel collocation method. Similar to chapter two, we also provide error estimate for the numerical solution. Some applications such as pattern formation in the Brusselator system and excitable media in FitzHughNagumo model are also studied.
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Chapter 1

Introduction

Radial basis function has been developed to solve partial differential equation for more than two decades. E.J. Kansa (Kansa, 1986; Kansa, 1990a; Kansa, 1990b) is the one who first solve the partial differential equation by multi-quadrics. People then start to develop radial basis function method for solving partial differential equations.

1.1 Radial function

The definition of radial function is easy and clear.

Definition 1. A function $\varphi : \mathbb{R}^d \mapsto \mathbb{R}$ is said to be radial provided there exists a univariate function $\phi : [0, +\infty) \mapsto \mathbb{R}$ such that

$$\varphi(x) = \phi(r), \quad \text{where } r = ||x||,$$

where $|| \cdot ||$ denotes some norm in $\mathbb{R}^d$. In this work, Euclidean norm will be used.

The term ”radial” is due to the property that $||x|| = ||y||$ gives $\varphi(x) = \varphi(y)$. Table 1.1 list out some classical radial functions. Multiquadric (MQ) is often used in many numerical methods for solving partial differential equations. Normally, Gaussian and multiquadric will be used in this thesis. The reason
<table>
<thead>
<tr>
<th>Name of radial function</th>
<th>$\phi(r), r \geq 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian (GA)</td>
<td>$e^{-(\varepsilon r)^2}$</td>
</tr>
<tr>
<td>Multiquadric (MQ)</td>
<td>$\sqrt{1 + (\varepsilon r)^2}$</td>
</tr>
<tr>
<td>Inverse Multiquadric (IMQ)</td>
<td>$\frac{1}{1 + (\varepsilon r)^2}$</td>
</tr>
<tr>
<td>Inverse quadratic (IQ)</td>
<td>$\frac{1 + (\varepsilon r)^2}{1 + (\varepsilon r)^2}$</td>
</tr>
<tr>
<td>Generalized Multiquadric</td>
<td>$(1 + (\varepsilon r)^2)^\beta$</td>
</tr>
<tr>
<td>Thin plate spline (TPS)</td>
<td>$r^2 \log(r)$</td>
</tr>
<tr>
<td>Generalized Thin plate spline</td>
<td>$r^{2k} \log(r)$</td>
</tr>
<tr>
<td>Matérn function</td>
<td>$\frac{K_{\beta-d/2}(\varepsilon r)(\varepsilon r)^{\beta-d/2}}{2^{\beta-1} \Gamma(\beta)}, \beta &gt; \frac{d}{2}$</td>
</tr>
</tbody>
</table>

Table 1.1: List of some radial functions. For the Matérn function, $K_\nu$ is the modified Bessel function of order $\nu$.

The choice of Gaussian as our basis function is because a stable solver has been developed when using Gaussian. Detailed discussion will be given in section 1.4. Generally speaking, for an interpolation problem (given a set of function values $\{f(x_1), f(x_2), \ldots, f(x_M)\}$) by using radial basis function (RBFs), a set of trial points (RBF centers) $\Xi = \{\xi_1, \xi_2, \ldots, \xi_N\}$ should be specified at first. Let $K(x, y) = \varphi(\|x - y\|)$ be the symmetric (strictly) positive definite kernel function with radial function $\varphi$. The trial space $U_{K,\Xi} = \text{span}\{K(\cdot, x) : x \in \Xi\}$ is then constructed for the approximation. In other words, an approximation has the form

$$U(x) = \sum_{\xi_j \in \Xi} \lambda_j K(x, \xi_j).$$

(1.1)

In order to solve for $\lambda_j, j = 1, \ldots, N$, it is necessary to set up a set of collocation points (Test points) $X = \{x_1, x_2, \ldots, x_M\}$ so that the equalities

$$U(x_i) = f(x_i), \quad i = 1, \ldots, M$$

(1.2)
are satisfied. The equalities (1.1) generate a linear system

\[
\begin{bmatrix}
K(x_1, x_1) & K(x_1, x_2) & \ldots & K(x_1, x_N) \\
K(x_2, x_1) & K(x_2, x_2) & \ldots & K(x_2, x_N) \\
\vdots & \vdots & \ddots & \vdots \\
K(x_M, x_1) & K(x_M, x_2) & \ldots & K(x_M, x_N)
\end{bmatrix}
\begin{bmatrix}
\lambda_1 \\
\lambda_2 \\
\vdots \\
\lambda_N
\end{bmatrix}
=
\begin{bmatrix}
f(x_1) \\
f(x_2) \\
\vdots \\
f(x_M)
\end{bmatrix}
\]

(1.3a)

or

\[
K(X, \Xi) \lambda = f(X).
\]

(1.3b)

The interpolant \( U \) is obtained by solving the linear system (1.3). However, the kernel matrix (interpolation matrix) \( K(X, \Xi) \) is normally ill-conditioned due to small gap between two neighboring centers or collocation points. Several strategies have been developed to overcome this behaviour. For instance, ill-conditioning can be avoided by selecting the trial space properly (Ling and Schaback, 2009).

### 1.2 Error Estimate

For the interpolation by radial basis function, an error estimate can be obtained in terms of its native space. This give rise to measure and guarantee the performance of approximation.

**Definition 2.** Let \( K \) be a symmetric strictly positive definite kernel. Let \( H_K = \text{span}\{K(\cdot, y) : y \in \Omega\} \) be a pre-Hilbert space with the inner product \( \langle \cdot, \cdot \rangle \) defined as

\[
\langle \sum_{j=1}^{N_K} c_j K(\cdot, x_j), \sum_{k=1}^{N_K} d_k K(\cdot, y_k) \rangle = \sum_{j=1}^{N_K} \sum_{k=1}^{N_K} c_j d_k K(x_j, y_k).
\]

The native space \( \mathcal{N}_K(\Omega) \) is defined as the completion of \( H_K(\Omega) \).

**Definition 3.** Let \( \mathcal{X} \) be a subset of \( \Omega \). The fill distance is defined as

\[
h_{\mathcal{X}, \Omega} = \sup_{x \in \Omega} \min_{x_j \in \mathcal{X}} \| x - x_j \|_2.
\]
Theorem 4 ((Fasshauer, 2007) Theorem 14.6). Suppose $\Omega \subseteq \mathbb{R}^s$ is open and bounded and satisfies an interior cone condition. Suppose $\Phi \in C^{2k}(\Omega \times \Omega)$ is symmetric and strictly conditionally positive definite of order $m$ on $\mathbb{R}^d$. Denote the interpolant to $f \in N_\Phi(\Omega)$ on the $(m-1)$-unisolvent set $\mathcal{X}$ by $P_f$. Fix $\alpha \in \mathbb{N}_0^s$ with $|\alpha| \leq k$. Then there exist positive constants $h_0$ and $C$ (independent of $x$, $f$ and $\Phi$) such that

$$|D^\alpha f(x) - D^\alpha P_f(x)| \leq C h^{k-|\alpha|} \sqrt{C_\Phi(x)} |f|_{N_\Phi(\Omega)},$$

provided $h_{\mathcal{X},\Omega} \leq h_0$. Here

$$C_\Phi(x) = \max_{|\beta|=2k} \max_{w \in \Omega \cap B(x, c_2 h_{\mathcal{X},\Omega})} |D_2^\beta \Phi(w, 0)|$$

with $B(x, c_2 h_{\mathcal{X},\Omega})$ denoting the ball of radius $c_2 h_{\mathcal{X},\Omega}$ centered at $x$.

Theorem 4 gives an error estimate for both interpolation and derivative approximation by using finite smoothness RBFs. For the error bound for RBFs with infinitely smoothness such as Gaussian or Multiquadric, please see (Fasshauer, 2007; Schaback, 1995a). Decreasing the fill distance $h_{\mathcal{X},\Omega}$ (increasing the number of centers $\mathcal{X}$ in $\Omega$) can reduce the absolute error. However, the absolute error will not goes to zero as the fill distance goes to zero. This is because decreasing the fill distance for well-distributed data will increase the instability to the kernel matrix $K$. This is the trade-off principle for RBF methods (Schaback, 1995a).

1.3 Trade-off principle

For solving the interpolation problem, the kernel matrix is normally ill conditioned. The condition number of the positive definite kernel matrix is given by

$$\text{cond}(K) = \|K\|_2 \|K^{-1}\|_2 = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}},$$

where $\lambda_{\text{max}}$ and $\lambda_{\text{min}}$ is the largest and smallest eigenvalue of $K$, respectively.
The upper bound for $\lambda_{\text{max}}$ can be obtained easily by the property of positive definiteness of $K$. On the other hand, the lower bound for the $\lambda_{\text{min}}$ is also proven for different type of RBFs (Wendland, 2004; Fasshauer, 2007; Schaback, 1995a; Madych and Nelson, 1992; Narcowich and Ward, 1992; Narcowich and Ward, 1991; Ball et al., 1992; Wu and Schaback, 1993).

For instance, the interpolation matrix of Gaussian $\Phi(x) = e^{-\varepsilon^2 \|x\|^2}$ has the lower bound

$$\lambda_{\text{min}} \geq C_s (\sqrt{2}\varepsilon)^{-s} e^{-40.71s^2/(q\varepsilon)^2} q_s^{-s},$$

where $M_s = 12 \left( \frac{\pi^{(s+2)} e}{9} \right)^{1/(s+1)} \leq 6.38s$ and $C_s = \frac{1}{2\Gamma \left( \frac{s+2}{2} \right)^{s}}$. 

In the lower bound of $\lambda_{\text{min}}$ (1.4), $q_s = \frac{1}{2} \min_{i \neq j} \|x_i - x_j\|_2$ denotes the separation distance. For fixed shape parameter $\varepsilon$, reducing the the fill distance for well-distributed data points will also reduce the separation distance. Therefore, the lower bound of the smallest eigenvalue $\lambda_{\text{min}}$ tends to zero exponentially. Hence, the condition number of $K$ will increase exponentially as the separation distance tends to zero. The accuracy cannot be improved by adding more centers. This is the trade-off principle for scattered-data interpolation (Schaback, 1995a).

On the other hand, with the fixed data set, the best accuracy will also be obtained with small shape parameter $\varepsilon$ (Madych, 1992). Similar to the above discussion, reducing the shape parameter will increase the condition number of the kernel matrix. Therefore, a wrong solution is obtained due to the instability.

### 1.4 RBF-QR

As in most of radial basis function methods, the best accuracy is often obtained when the RBF is relatively flat, i.e., very small shape parameter $\varepsilon$ (Madych, 1992). However, the typical trade-off principle in RBF methods (Wendland, 2004; Schaback, 1995a) stated that the stability will decrease as accuracy increases. This is because the kernel matrix will become ill-conditioned when the
RBF is flattened. However, for the Gaussian kernel, a stable solver which was called RBF-QR were developed to overcome the instability due to flat RBF (Fornberg et al., 2011; Fasshauer and McCourt, 2012). RBF-QR with Bessel kernel can also be obtained in (Fornberg et al., 2011) in a similar way.

General speaking, let \( K(x, x_j) = \phi(\varepsilon \|x - x_j\|_2) \) be the kernel at center \( x_j \). The instability of the kernel matrix \( K_{ij} = K(x_i, x_j) \) is normally due to the shape parameter. RBF-QR transforms the basis from the original kernel to a set of new basis which is insensible to small \( \varepsilon \). For detailed discussion, please see section 2.4.2.

1.5 Thesis overview

In this thesis, We begin with solving the diffusion equation on folded surfaces. In this section, generalized finite difference together with closest point extension is used to solve PDEs on surface. Power function allowed one to estimate the relative error in advance. Convergence study will be provided to justify the a priori error estimate. Numerical demonstration for flat-top sphere and punch-in sphere are also provided. Next, Chapter 3 will study the convergence of the both constrained least square(CLS) Kansa’s method and weighted least-square(WLS) Kansa’s method in \( H^2 \) norm. Error analysis for both methods are provided. Numerical demonstration are provided to verify the error estimate for several cases. In Chapter 4, we solve partial differential equations on smooth surface with a new embedding method. The embedding method is high order accurate and the numerical solution is solved by least-squares kernel collocation method. Error analysis and numerical verification for this numerical solution are also provided.
Chapter 2

Diffusion equation on folded surfaces or curves with corners.

2.1 Introduction to Closest point method

Partial differential equations (PDEs) on surfaces arise in a variety of application areas including biological systems, medical imaging, fluid dynamics, mathematical physics, image processing and computer graphics. In this chapter, localized meshless method is used to solve diffusion on smooth and folded surfaces. Curves with corners will also be investigated.

A variety of numerical methods have been proposed to approximate the solution of partial differential equations on surfaces. These include discretizations on parameterized surfaces, finite difference and finite element methods on triangulated surfaces, and embedding methods.

Each class of methods is characterized by certain advantages and disadvantages. Parametrization methods can be very efficient, but these methods require a parametrization of the surface. Typically, the construction of a parameterization leads to distortions in the surface as well as singularities (Floater and Hormann, 2005; Lui et al., 2005; Stam, 2003; Witkin and Kass, 1991). We may avoid this complication by discretizing on triangulated surfaces. Unfortunately, finite difference discretizations on triangulated surfaces are more
difficult to construct on curved surfaces than on the plane and it can be difficult to compute geometric quantities such as the curvature and the normal to the surface (Bertalmio et al., 2001; Greer, 2006; Turk, 1991). On the other hand, finite element methods on triangulated surfaces can be effective when applied to problems of elliptic or parabolic type (Dziuk, 1988; Dziuk and Elliott, 2007).

In the embedding class of methods, the surface and the corresponding surface PDE are represented in the underlying \( d \)-dimensional embedding space (e.g., a problem posed on a two-dimensional curved surface might be represented and solved in a three-dimensional neighbourhood of the surface) thereby enabling the use of standard Cartesian grid methods in \( \mathbb{R}^d \). The most popular finite difference (Bertalmio et al., 2001; Greer, 2006) and RBF discretizations (Flyer and Wright, 2009; Fuselier and Wright, 2012) of this type project the surface Laplacian to the tangent space of the surface. Often, a level set representation of the surface is used, in which case there is no direct generalization to open surfaces or surfaces without orientation. Moreover, embedding methods typically introduce artificial boundary conditions at the boundary of the computational domain, leading to an addition error and first-order accuracy for diffusion problems. These complications can be overcome by using the closest point method (Ruuth and Merriman, 2008), which is a high-order accurate method that embeds the surface within the Euclidean embedding space by means of a closest point mapping. The standard explicit closest point method is comprised of an evolution step and an interpolation step: the method must interpolate function values on the surface at each time step in order to replace derivatives intrinsic to the surface with standard Cartesian operators.

In (Piret, 2012), Piret proposed to discretize the closest point method using radial basis functions. As a consequence of using radial basis functions, the method is not restricted to Cartesian grids. This allows for two fundamental advantages over the standard closest point method. First, it is straightforward to use irregular or refined grids according to the needs of the problem. Second, the freedom of selecting nodal points naturally allows one to eliminate the in-
terpolation step of the closest point method by making an appropriate node selection. By avoiding the interpolation step, the computational error and cost associated with interpolation is eliminated. The method proposed in this paper also combines the closest point method and the radial basis function projection method to solve PDEs on surfaces. As in Piret’s approach, our approach does not involve an interpolation step, thereby eliminating a source of error and opening the possibility of significant savings in computational cost. Apart from this, we will show that our proposed method is error optimal, i.e., the spatial approximation has a minimal error bound among all meshless methods. Moreover, the error bound is of a-priori type: it depends only on the distribution of nodes and the type of kernel or basis function. On the other hand, the discretization of the spatial variables in our approach leads to a differentiation matrix $W$ such that $u_t = Wu$. While the differentiation matrix $W$ is error optimal, it is also very ill-conditioned when the radial basis functions become flat or when the nodal points are very dense. Consequently, as we refine our discretization, the differentiation matrix becomes ill-conditioned (Larsson and Fornberg, 2003b; Fornberg and Wright, 2004; Larsson and Fornberg, 2003a). This trade-off is inherent in meshless methods. See (Fornberg et al., 2011; Larsson et al., 2013) for a strategy to handle the ill-conditioning by changing the basis function to an orthogonal basis, thereby stabilizing the computation for flat radial basis functions. Throughout this paper, the differentiation matrix $W$ arising in numerical experiments is solved by this RBF-QR strategy.

In addition to the development of an error-optimal RBF discretization, this paper introduces a generalization of the closest point method appropriate for diffusion on folded surfaces. The standard closest point method is built on the assumption that the closest point function is sufficiently smooth within the computational band. As a consequence, the standard method cannot be used to compute the solutions of PDEs on curves with corners or surfaces with folds. In (Rockstroh et al., 2012), a transformation was introduced to give a smooth, transformed problem which is amenable to computation via the
standard closest point method. Unfortunately, the transformed problem has increased dimensionality, and consequently is computationally expensive. In this paper, we develop an extension of the closest point method for solving diffusion on curves with corners and on folded surfaces. The method computes within the original embedding space and uses node placement along the folds. This makes a radial basis function discretization particularly appropriate. Numerical experiments demonstrate that the proposed method retains high-order accuracy for smooth curves and surfaces, while giving first order convergence for computations on geometries with folds.

2.2 Surface Embedding

The closest point method, originally proposed by Ruuth and Merriman (Ruuth and Merriman, 2008) is an embedding method for solving PDEs on surfaces. The method embeds the surface operator to the Euclidean space $\mathbb{R}^n$ using a closest point mapping. Such an embedding is called a closest point extension. By alternating the closest point extension with a traditional PDE solver on $\mathbb{R}^n$, we can obtain an explicit method for solving a surface PDE in the embedding space.

Let $S \subset \mathbb{R}^n$ be a smooth surface and $\nabla$ be the standard Euclidean gradient in $\mathbb{R}^n$. Then, the surface gradient, denoted by $\nabla_S$, is defined as:

$$\nabla_S := \nabla - \hat{n}(\hat{n} \cdot \nabla), \quad (2.1)$$

where $\hat{n}$ is the unit normal to the surface $S$. Consider a $C^1$ vector field $\phi : \mathbb{R}^n \rightarrow \mathbb{R}^n$ that is constant along the normal direction to $S$. The directional derivative satisfies

$$0 = \frac{d}{d\hat{n}} (u \circ \phi) = \hat{n} \cdot \nabla(u \circ \phi),$$

which we combine with (2.1) to obtain

$$\nabla_S(u \circ \phi) = \nabla(u \circ \phi) - \hat{n} \cdot \nabla(u \circ \phi) \hat{n} = \nabla(u \circ \phi), \quad \text{on } S. \quad (2.2)$$
Thus, for any $C^1$ function that is constant along the normal direction to $S$, we observe that, on the surface, standard Euclidean gradients (defined on the embedding space) coincide with the desired surface gradients. A particularly convenient vector field $\phi : \mathbb{R}^n \rightarrow S$ is the closest point mapping

$$\phi_S(x) = \arg \min_{s \in S} |x - s|, \text{ for all } x \in \mathbb{S},$$

where $\mathbb{S} \subseteq \mathbb{R}^n$ is a neighborhood of $S$ over which the closest point mapping $\phi_S$ is $C^1$. Generally, the maximum possible $\mathbb{S}$ is determined by the curvature of $S$. For any $C^1$ surface, we can properly embed $S \subset \mathbb{S}$. For example, if $S \in \mathbb{R}^2$ is circle, then the maximum possible $\mathbb{S}$ will be the whole plane $\mathbb{R}^2$ except the center of $S$.

Similar conditions can be derived for the surface divergence for any differentiable vector field $\varphi : \mathbb{R}^n \rightarrow \mathbb{R}^n$. The surface divergence operator, denoted by $\nabla_S$, is defined as:

$$\nabla_S \varphi = \left( \nabla - \hat{n} \hat{n} \cdot \nabla \right) \cdot (\varphi - \hat{n} \hat{n} \cdot \varphi)$$

$$= \nabla \cdot \varphi - \hat{n} \nabla \varphi \cdot \hat{n} - \hat{n} \cdot \varphi \nabla \cdot \hat{n},$$

where $\hat{n}$ is the unit normal to the surface $S$. Similarly, if $\varphi$ is tangent to the surface and all the surfaces displaced by a fixed distance from $S$, then the surface divergence of $\varphi$ coincides with the usual divergence at the surface

$$\nabla_S \cdot \varphi = \nabla \cdot \varphi, \text{ on } S.$$

A combination of these two principles demonstrates that we may evaluate the traditional Laplacian $\Delta(u \circ \phi_S) = \nabla \cdot \nabla (u \circ \phi_S)$ in $\mathbb{S}$ instead of the surface Laplacian $\Delta_S(u \circ \phi_S) = \nabla_S \cdot \nabla_S (u \circ \phi_S)$ on $S$ for $u \in C^2$. In fact, any nonlinear diffusion operator can be embedded to a traditional one in $\mathbb{S}$; see (Ruuth and Merriman, 2008).
Figure 2.1: A schematic demonstration for a data point $x_i$ on surfaces $\mathcal{S} \subset \mathbb{R}^2$ along with its symmetric 3-point local neighbourhood $X_i$ and $\mathcal{S}$-orthogonal extension $\overline{X}_i$.

### 2.3 $\mathcal{S}$–Orthogonal Data Distribution

For the sake of clarity, let $u_\mathcal{S}$ be the restriction to the surface $\mathcal{S}$ for any function $u$ defined on $\mathbb{R}^n$. Consider the heat equation intrinsic to the surface $\mathcal{S}$, i.e.,

$$\partial_t u_\mathcal{S} = \Delta_\mathcal{S} u_\mathcal{S} \text{ on } \mathcal{S}. \quad (2.6)$$

After embedding the surface PDE to $\overline{\mathcal{S}}$, we get an embedded PDE:

$$\partial_t u = \Delta(u \circ \phi_\mathcal{S}) \text{ in } \overline{\mathcal{S}}. \quad (2.7)$$

We can use any solver developed for the embedded PDE posed on $\mathbb{R}^n$ to solve the surface PDE (2.6).

Meshless methods are methods that do not require any mesh structure. When applied to the closest point method with an appropriate mesh, meshless methods give a trivial discretization of the closest point extension step. In this work, we adopt the localized meshless approach in (Cecil et al., 2004; Li et al., 2013; Piret, 2012; Shu et al., 2003; Tolstykh, 2000; Wright, 2003).

First, let $X = \{x_i\}_{i=1}^N \subset \mathcal{S}$ be the set of data points used to discretize $\mathcal{S}$; see Figure 2.1 for a schematic demonstration. Using the set of normal vectors...
\( \mathbf{n}(\mathbf{X}) = \{ \hat{n}(x_i) : x_i \in \mathbf{X} \} \), the set \( \mathbf{X} \) can be extended to a discretization for \( \overline{\mathbf{S}} \).

We define \( G_h(\mathbf{X}) : \mathcal{S} \rightarrow \overline{\mathbf{S}} \) such that

\[
G_h(\mathbf{X}) = \mathbf{X} + h \mathbf{n}(\mathbf{X}) = \{ x_i + h \hat{n}(x_i) : x_i \in \mathbf{X}, h \in \mathbb{R} \}.
\]

It is easy to see that \( G_h(\mathbf{X}) \) is a set of points extended from \( \mathbf{X} \) by a distance \( h \) along its normal direction \( \mathbf{n}(\mathbf{X}) \). For simplicity, assume \( h > 0 \) is sufficiently small (w.r.t. \( k \)) such that, \( \mathcal{G} : \mathcal{S} \rightarrow \overline{\mathbf{S}} \) and

\[
\overline{\mathbf{X}} = \mathcal{G}(\mathbf{X}) := \mathbf{X} \cup G_{\pm h}(\mathbf{X}) \cup \cdots \cup G_{\pm kh}(\mathbf{X}) \subset \overline{\mathbf{S}}. \tag{2.8}
\]

With \( N = |\mathbf{X}| \) points on \( \mathcal{S} \), we now have a set of \( M = (2k + 1)N \) data points in \( \overline{\mathbf{S}} \). By construction, trivially, we also have a discretized closest point mapping (2.3), that maps \( u_{|\mathbf{X}} \rightarrow u_{|\overline{\mathbf{X}}} \). The tradeoff is that the data points in \( \overline{\mathbf{X}} \) are not regular.

### 2.3.1 Point distribution for corners and folded surfaces

Suppose for now that our surface \( \mathcal{S} \) is nonsmooth and \( \mathcal{S} = \bigcup \mathcal{S}_j \), where each \( \mathcal{S}_j \) is smooth. Define the singular curve \( \Gamma \) to be the intersection of these subsurfaces, i.e., the set on which \( \mathcal{S} \) is nonsmooth. It is desirable to have data on \( \Gamma \) to enhance the resolution of the numerical approximation. We now describe mesh selection on singular surfaces. For each data point \( x_i \in \mathbf{X} \subset \mathcal{S} \), we either have \( x_i \) inside a smooth subsurface or on the singular curve. For \( x_i \in \mathcal{S}_j \setminus \partial \mathcal{S}_j \) (for some \( j \)), its local neighbourhood should be restricted to the same subsurface; i.e., \( X_i \subset \mathcal{S}_j \). This local neighbourhood can then be extended in the \( \mathcal{S} \)-orthogonal direction to yield \( \overline{X}_i \).

Now, for \( x_i \in \Gamma \), \( x_i \) must belong to two or more smooth subsurfaces. That is, \( x_i \in \mathcal{S}_{i1} \cap \cdots \cap \mathcal{S}_{ik} \subseteq \Gamma \) where \( k \geq 2 \). Notice that our discretization requires smoothness of the closest point function in a band around each subsurface, a requirement that can be satisfied by taking \( h \) sufficiently small. This contrasts with the original closest point method that places a more strict, global restriction over \( \mathcal{S} \). Figure 2.2 gives a simple case of two smooth curves meeting at a
corner point $x_i$. At the corner point $x_i$, asymmetric local neighbourhoods are used to satisfy $X_{i1} \subset S_1$ and $X_{i2} \subset S_2$. In our method, these local neighbourhoods will lead to multiple sets of weighings for the corner $x_i$. An arithmetic average will be taken as the final weighting.

Note that the $S$-orthogonal extensions $\overline{X_{i1}}$ can extend past subsurface $S_2$, and vice versa for an acute angled corner with our method. These overlapping grids will not cause any trouble for our method.

Figure 2.3(a) shows an example of a dented sphere $S \subset \mathbb{R}^3$ composed of $S_1$, a part of the unit sphere, and $S_2$, the dented top. Figure 2.3(b) is a bird’s-eye view of some data points $X$ near a part of $\Gamma$. In this projected view, the outer annular region belongs to $S_1$ and the inner region belongs to $S_2$. $S_1$ and $S_2$ meet at $\Gamma$ (represented by the solid line). For a data point $x_i \in S_1 \cap S_2$, $\overline{X_{i1}}$ and $\overline{X_{i2}}$ are obtained via neighborhood searches. See Figures 2.3(b) and 2.3(c) for illustrations of these sets.

### 2.3.2 Reduced semi-discrete form

For each $x_i \in X \subset S$ and some $\varepsilon > 0$, let the $i^{th}$ local neighbourhood be denoted by $X_i = \{x \in X \subset S : |x - x_i| < \varepsilon\}$. Then, this neighbourhood
Figure 2.3: A nonsmooth manifold in $\mathbb{R}^3$ and a schematic data point distribution.
on $\mathcal{S}$ can be extended to $\overline{\mathcal{S}}$ by $\overline{\mathbf{X}}_i = G(\mathbf{X}_i) \subset \overline{\mathbf{X}}$. Assuming we have a set of generalized finite-difference weightings $w_{ij} \in \mathbb{R}$, such that for each $\mathbf{x}_i \in \mathbf{X}$,

$$Lu(\mathbf{x}_i) \approx \sum_j w_{ij} u(\boldsymbol{\xi}_j), \quad \boldsymbol{\xi}_j \in \overline{\mathbf{X}}_i,$$

(2.9)

where $L$ is a linear functional. For data $x_i \in \Gamma$ on the surface singularity, the linear combination in (2.9) involves all points $\boldsymbol{\xi}_j \in \overline{\mathbf{X}}_i \cup \cdots \cup \overline{\mathbf{X}}_k$. A detailed discussion on the generalized finite-difference method is presented in the next section. For now, suppose (2.9) is available for all data points in $\mathbf{X}$. Collecting all these weights in an $M \times M$ sparse matrix $W$, as in the standard finite difference method, we obtain a semi-discrete formulation,

$$\partial_t u(\overline{\mathbf{X}}) = W(u \circ \phi_S)(\overline{\mathbf{X}}).$$

(2.10)

Advancing (2.10) via any time discretization scheme will yield a set of new nodal values at all points in $\overline{\mathbf{X}}$. For simplicity, we consider the forward Euler scheme which yields

$$u(\overline{\mathbf{X}}, t + \Delta t) = (u \circ \phi_S)(\overline{\mathbf{X}}, t) + \Delta t W(u \circ \phi_S)(\overline{\mathbf{X}}, t).$$

(2.11)

It remains to discretize the closest point mapping $u \circ \phi_S$. This will yield a standard difference equation to update the approximate solution of the embedded PDE (2.7).

Recall that our target is the surface PDE (2.6) rather than the embedded (2.7). In other words, we are only interested in the function values of $u \circ \phi_S$ or, equivalently, $u$ values at points $\mathbf{X}$ belonging to $\mathcal{S}$. Those at points $\overline{\mathbf{X}} \setminus \mathbf{X}$ are specified by the closest point mapping, i.e., $u \circ \phi_S(\overline{\mathbf{X}}) = u(G^{-1}(\overline{\mathbf{X}}))$. Notice, however, that our data points give the function values outside $\mathcal{S}$ as copies of those on the surface. Thus, in (2.11), the values of $u(\overline{\mathbf{X}} \setminus \mathbf{X})$ and the corresponding weightings in $W$ are unnecessary. Applying this observation, the closest point mapping can be written in matrix form as

$$(u \circ \phi_S)(\overline{\mathbf{X}}, t) = E u(\mathbf{X}, t), \quad \text{for } E = \mathbf{1} \otimes I_N \in \{0, 1\}^{M \times N},$$
where $\otimes$ is the kronecker product and $E$ is an upsampling with the $(2k+1)$ vector $1$ of all ones, assuming points in $X$ are listed first in $\overline{X}$ as in (2.8). We also define the corresponding downsampling $E^\dagger = e_1^T \otimes I_N \in \{0,1\}^{N \times M}$ that extracts values at $X$. Applying operators $E$ and $E^\dagger$, the $M \times M$ system (2.11) can be reduced to an $N \times N$ system:

$$u(X, t + \Delta t) = E^\dagger u(\overline{X}, t + \Delta t),$$

$$= E^\dagger((u \circ \phi_S)(\overline{X}, t) + \Delta t W (u \circ \phi_S)(\overline{X}, t)),$$

$$= E^\dagger(Eu(X, t) + \Delta t W Eu(X, t)),$$

$$= (I_N + \Delta t E^\dagger W E) u(X, t),$$

(2.12)

where the $N \times N$ matrix $E^\dagger WE$ only requires $N$ sets of finite difference weights $w_{ij}$, given by (2.9), for the points $X$ instead of all $M$ sets for $\overline{X}$.

Equation (2.12) gives the forward Euler approximation of the time discretization of the surface PDE $\partial_t u_S = \mathcal{L}_S u_S$, (2.6), on data points $X \subset S$. Other time-stepping methods may also be considered. Similar to the forward Euler case, such methods should be applied to the reduced semi-discrete form for the surface PDE,

$$\partial_t u_S(X) = (E^\dagger WE) u_S(X).$$

(2.13)

### 2.4 Norm-Optimal Approximation

We now address how the generalized finite difference weightings (2.9) can be obtained for all $x_i \in X \subset S$ to evaluate the matrix $E^\dagger WE$ in the reduced semi-discrete surface PDE (2.13). Recall that $x_i \in X$ is any given data point on the surface $S$. The subset of neighboring points $X_i \in S$ of $x_i$ is then obtained by some neighborhood search technique over the set $X$, such as a kd-tree search. Then, the subset $\overline{X}_i \subset \overline{X}$ is obtained by extending points in the normal direction, as in (2.8), and we denote $n_i = |\overline{X}_i|$. Throughout this section, the index $i$ will be used to denote the current point under consideration and will be omitted when no ambiguity arises. Generally speaking, we need a
method to look for the weighting \(\{w_{ij}\}\) in (2.9) such that the linear functional \(\delta_{x_i}\mathcal{L}\) is well-approximated by a linear combination of the function values of \(u\) at \(\overline{X}_i\),

\[
\delta_{x_i}\mathcal{L}[u] = \mathcal{L}u(x_i) \approx \sum_j w_{ij} u(\xi_j), \quad \xi_j \in \overline{X}_i. \tag{2.14}
\]

Equivalently, in matrix form, it suffices to find the matrix \(W\) in the following linear system

\[
\mathcal{L}u(X) \approx E^\dagger W u(X),
\]

where \(E^\dagger W\) is of size \(N \times M\) with entries \([E^\dagger W]_{ij} = w_{ij}\) in (2.14). For the singular points \(x_i \in \Gamma\), the linear functional \(\delta_{x_i}\mathcal{L}\) has multiple approximations, one for each subsurface to which \(x_i\) belongs.

To select the weighting so that the discretization on a set of given nodes is error optimal, we introduce a reproducing kernel Hilbert space. As will be shown, \textit{a priori} error estimation is possible with our approach.

Let \(K : \Omega \times \Omega \to \mathbb{R}\) be a symmetric, strictly positive definite kernel with \(\Omega \supset \overline{X}_i\) and let \(H_K(\Omega) = \text{span}\{K(\cdot, y) : y \in \Omega\}\). We define an associated bilinear form \((\cdot, \cdot)_K\) for \(H_K\) by

\[
\left\langle \sum_j c_j K(\cdot, x_j), \sum_k d_k K(\cdot, y_k) \right\rangle_K = \sum_j \sum_k c_j d_k K(x_j, y_k).
\]

Thus, \(H_K(\Omega)\) is a pre-Hilbert space with \((\cdot, \cdot)_K\) as an inner product. Completion of \(H_K(\Omega)\) yields a Hilbert space which is called the native space, denoted by \(\mathcal{H}(\Omega)\) for simplicity. The space \(\mathcal{H}(\Omega)\) satisfies

\[
K(x, y) = \langle K(x, \cdot), K(y, \cdot) \rangle_{\mathcal{H}},
\]

\[
f(x) = \langle f, K(x, \cdot) \rangle_{\mathcal{H}},
\]

\[
\langle \delta_x \mathcal{L}, \delta_x \mathcal{L} \rangle_{\mathcal{H}^*} = \delta_x \mathcal{L}^x \delta_x \mathcal{L}^y K(x, y) = \mathcal{L}^x \mathcal{L}^y K(x_i, x_j),
\]

for all \(x, y \in \Omega\), \(f \in \mathcal{H}\) and \(\delta_x \mathcal{L} \in \mathcal{H}^*\), where \(\mathcal{H}^*\) is the dual space of \(\mathcal{H}\) and the superscript in \(\delta_x \mathcal{L}^x\) is used to emphasize its action on the first variable of \(K(x, y)\).
Suppose we want to find the weights in (2.9) to minimize the absolute error (Schaback, 2013). The approximation error is given by

$$|L(u(x_i) - \sum_{\xi_j \in X} w_j u(\xi_j)| = \left| \left( \delta_{x_i} \mathcal{L} - \sum_{\xi_j} w_j \delta_{\xi_j} \right)[u] \right|,$$

$$\leq \left\| \delta_{x_i} \mathcal{L} - \sum_{\xi_j} w_j \delta_{\xi_j} \right\|_{\mathcal{H}^*} \left\| u \right\|_{\mathcal{H}^*}$$

(2.15)

where $w_j := w_{ij}$ is the weight in (2.9). We define the power function $\epsilon_{\delta_{x_i} \mathcal{L}, X_i, w} := \delta_{x_i} \mathcal{L} - \sum w_j \delta_{\xi_j}$ for a linear functional $\delta_{x_i} \mathcal{L}$, node point $X_i$, and weighting $w$. Note that the square of the norm of the power function is a bilinear form such that:

$$P^2(w) := \left\| \epsilon_{\delta_{x_i} \mathcal{L}, X_i, w} \right\|_{\mathcal{H}^*}^2 = \left\| \delta_{x_i} \mathcal{L} - \sum_{\xi_j \in X_i} w_j \delta_{\xi_j} \right\|_{\mathcal{H}^*}^2,$$

$$= \langle \delta_{x_i} \mathcal{L}, \delta_{x_i} \mathcal{L} \rangle_{\mathcal{H}^*} - 2 \sum w_j \langle \delta_{x_i} \mathcal{L}, \delta_{\xi_j} \rangle_{\mathcal{H}^*} + \sum \sum w_j w_k \langle \delta_{x_i}, \delta_{\xi_j} \rangle_{\mathcal{H}^*},$$

$$= \mathcal{L}^x \mathcal{L}^y K(x_i, x_i) - 2 \sum w_j \mathcal{L}^x K(x_i, x_j) + \sum \sum w_j w_k K(x_k, x_j).$$

(2.16)

Finding an error optimal formula is equivalent to minimizing $P^2$. It is easily shown that the solution $w^*$ of the following system minimizes $P^2$:

$$\sum_{x_j \in X_i} w^*_j K(x_k, x_j) = \mathcal{L}^x K(x_i, x_k), \quad x_k \in X_i.$$  

(2.17)

Equivalently, in matrix form a minimizer is obtained if $w^*$ satisfies

$$K(X_i, X_i) w^* = \mathcal{L}^x K(x_i, X_i).$$  

(2.18)

Applying this result to (2.16), we observe that the minimum of $P^2$ (i.e., the square of absolute error of (2.9) at the point $x_i$) is given by

$$\min_w P^2(w) = P^2(w^*) = \mathcal{L}^x \mathcal{L}^y K(x_i, x_i) - \sum_{x_j \in X_i} w^*_j \mathcal{L}^x K(x_i, x_j).$$

Consequently, the solution of (2.17) is the weighting such that the approximation (2.14) has the smallest error in the sense of the native space norm $\| \cdot \|_{\mathcal{H}}$. Note that the native space $\mathcal{H}$ is a reproducing kernel Hilbert space. For each type of kernel $K$, there is a corresponding native space $\mathcal{N}_K$. In our
problem, we take $K(x, y) = e^{-\left(\frac{1}{c}||x-y||_{2}\right)^2}$. For the Matérn kernel $K(x, y) := ||x-y||_{2}^{m-d/2}K_{m-d/2}\left(\frac{1}{c}||x-y||_{2}\right)$, $x, y \in \mathbb{R}^{d}$, where $K_{v}(r)$ is the modified Bessel function of the second kind, the corresponding native space is the Sobolev space $W_{2}^{m}(\mathbb{R}^{d})$ for $m > d/2$. For the native space of other kernels, see (Fasshauer, 2007; Wendland, 2004). In both cases, the shape parameter $c$ controls the shape of the kernel. The trade-off property for the radial basis function method (Schaback, 1995a; Schaback, 1995b) is that the accuracy improves as the shape parameter $c$ grows large or as the nodal point distribution becomes dense. Computationally, either case comes at the cost of more ill-conditioned matrices.

Once the kernel $K$ is fixed, one can directly compute the power function and error bound without any knowledge of the exact solution. Thus, we can obtain an error bound for a given node before computing any numerical solution. Note that the error bound (2.15) can also be interpreted as the relative error of the discretization in terms of the $H$-norm of the exact solution $u$.

2.4.1 The meshless finite difference method

The meshless finite difference method, a.k.a. the localized meshless method (Cecil et al., 2004; Shu et al., 2003; Tolstykh, 2000; Wright, 2003), has been developed for the same purpose to find the weighting $w$ in (2.14). Here, we shall show that the weighting found by the meshless finite difference method coincides in exact arithmetic with ours in (2.17).

Suppose we are given a set of data sites $\mathbf{X}_i$, but with unknown function values $u(\mathbf{X}_i)$. Meshless methods, with a suitable kernel function $K$, give an interpolant of $\tilde{u}$ in the form

$$\tilde{u}(x) = \sum_{x_j \in \mathbf{X}_i} w_j K(x, x_j).$$

Imposing interpolation conditions $\tilde{u} = u$ at all $x \in \mathbf{X}_i$, we express the weighting as

$$w = K(\mathbf{X}_i, \mathbf{X}_i)^{-1}u(\mathbf{X}_i),$$
where \( \mathbf{u}(\mathbf{X}_i) \) is a vector of (unknown) function values and the matrix entries are defined by \([K(\mathbf{X}_i, \mathbf{X}_i)]_{jk} = K(x_j, x_k)\) for \( x_j, x_k \in \mathbf{X}_i \). Note that the matrix \( K(\mathbf{X}_i, \mathbf{X}_i) \) is nonsingular provided the kernel \( K \) is positive definite.

The meshless finite difference method uses information from the interpolant to approximate the unknown function. For our discussion we have

\[
\mathcal{L}u(x_i) \approx \mathcal{L}\tilde{u}(x_i),
\]

\[
= \sum_{x_j \in \mathbf{X}_i} w_j \mathcal{L}^x K(x_i, x_j),
\]

\[
= (\mathcal{L}^x K(x_i, \mathbf{X}_i))^T \cdot \mathbf{w},
\]

\[
= (\mathcal{L}^x K(x_i, \mathbf{X}_i))^T K(\mathbf{X}_i, \mathbf{X}_i)^{-1} u(\mathbf{X}_i),
\]

\[
= \mathbf{w} \cdot \mathbf{u}(\mathbf{X}_i) = \sum_{x_j \in \mathbf{X}_i} w_j u(x_j).
\]

Therefore, the meshless finite difference method returns the solution of

\[
K(\mathbf{X}_i, \mathbf{X}_i)\mathbf{w} = \mathcal{L}^x K(x_i, \mathbf{X}_i),
\]

as the weighting \( \mathbf{w} \), which is identical to our previous results (2.17) and (2.18). Thus, the meshless finite difference method is error optimal. Note, however, that the reproducing kernel Hilbert space approach (Fasshauer, 2007; Schaback, 2013; Schaback, 2015) has the advantage of allowing us to measure error by using the corresponding power function.

### 2.4.2 Finding optimal-weights numerically

To numerically obtain the generalized finite difference weighting for point \( x_i \in \mathbf{X} \subset S \), we solve the \( n_i \times n_i \) matrix system (2.18). This gives an \( n_i = |\mathbf{X}_i| \) point interpolant over a neighbourhood of \( x_i \). For any commonly used global kernel, such as the Gaussian and Matérn kernels, the kernel matrix \( K := K(\mathbf{X}_i, \mathbf{X}_i) \) is full and, generally speaking, ill-conditioned. To solve (2.18) directly, it is necessary to invert the kernel matrix, which gives rise to numerical instability. In our numerical computation, we adopt the Gaussian kernel \( K(x, y) = e^{-(\frac{1}{2}\|x-y\|^2)} \) and apply the stable RBF-QR method by Fornberg et al. (Fornberg et al.,
Note that the method can also be applied to the Matérn kernel (Fornberg et al., 2009; Fornberg et al., 2011) in which case one will be working with error bounds in some standard Sobolev spaces, which are the native spaces of the Matérn kernel (Fasshauer, 2007).

It is not difficult to see why the matrix \( K(\mathbf{X}_i, \mathbf{X}_j) \) becomes ill-conditioned for large \( c \)-values. In the limit \( c \to \infty \), the Gaussian kernels become flat and form a numerically unstable basis. To avoid this problem, Gaussian radial basis functions may be changed to another set of stable basis functions sharing the same span. It is shown in (Fornberg et al., 2011) that the Gaussian kernel \( K(x, x_k) = e^{-\frac{1}{2}(\|x-x_k\|^2)} \) has an expansion in 2D,

\[
K(x, x_k) = \sum_{j=0}^{\infty} \sum_{m=0}^{\infty} d_{j,m} c_{j,m}(x_k) T_{j,m}(x) + \sum_{j=0}^{\infty} \sum_{m=1-p}^{\infty} d_{j,m} s_{j,m}(x_k) T_{j,m}^s(x),
\]

(2.19)

for \( 0 \leq m \leq \lfloor \frac{d}{2} \rfloor = \frac{d-1}{2} \) with \( p = \text{mod}_2 j \). In this expression, the functions

\[
T_{j,m}^c(x) = e^{-r^2/c^2} r^{2m} T_{j-2m}(r) \cos((2m+p)\theta), \quad \text{for } 2m+p = 0
\]

(2.20)

and

\[
T_{j,m}^s(x) = e^{-r^2/c^2} r^{2m} T_{j-2m}(r) \sin((2m+p)\theta), \quad \text{for } 2m+p \neq 0
\]

(2.21)

form a linearly independent set and are defined using the Chebyshev polynomials \( T_m(r) \) where \( x = (r, \theta) \) is the polar coordinate of \( x \). The coefficients in (2.19) depend on the point distribution of \( \mathbf{X}_i \) only and are given by

\[
d_{j,m} = e^{-2j} \left( \frac{j}{2} \right)^j \left( \frac{j+2m+p}{2} \right)^{j-m} \left( \frac{j-2m-p}{2} \right)^{j-m},
\]

\[
c_{j,m}(x_k) = b_{m+p} t_{j-2m} e^{-r^2/c^2} r_j^j \cos((2m+p)\theta_k),
\]

\[
s_{j,m}(x_k) = b_{m+p} t_{j-2m} e^{-r^2/c^2} r_j^j \sin((2m+p)\theta_k),
\]

where \( b_0 = 1 \) and \( b_m = 2, m > 0 \), \( t_0 = \frac{1}{2} \) and \( t_j = 1, j > 0 \). The function \( _1F_2 \) is the hypergeometric function with \( \alpha_{j,m} = \frac{j-2m+p+1}{2} \) and \( \beta_{j,m} = \left[ j - 2m + 1 \right] \).

Despite the complexity, if we truncate the infinite sum in (2.19) after \( J > n_i \) terms, the kernel matrix can be analytically decomposed as

\[
K(\mathbf{X}_i, \mathbf{X}_i)^T = CDV^T = (QR)DV^T,
\]

(2.22)
where $C = QR$ is an $n_i \times J$ matrix consisting of coefficients $c_{j,m}(\mathbf{x}_i)$ and $s_{j,m}(\mathbf{x}_i)$ and its full QR-factorization, $D$, is a $J \times J$ diagonal matrix consisting of entries $d_{j,m}$. The $n \times J$ matrix $V = V(\mathbf{x})$ consists of the functions $T^c_{j,m}(\mathbf{x})$ and $T^s_{j,m}(\mathbf{x})$.

The QR-factorization of the matrix $C$ gives $C = QR = Q[R_1 \quad R_2]$ where $R_1$ contains the left $n_i \times n_i$ block of $R$ and $R_2$ contains the remaining columns. Let $D_1$ be the $n_i \times n_i$ principal submatrix of the diagonal matrix $D$ and denote the remaining nonzero $(J - n_i) \times (J - n_i)$ submatrix by $D_2$. We observe that

$$Q^T K(\mathbf{x}_i, \mathbf{x}_j)^T = RDV^T,$$

$$= [R_1 \quad R_2] \left[ \begin{array}{c} D_1 \\ D_2 \end{array} \right] V^T,$$

$$= [R_1 D_1 \quad R_2 D_2] V^T,$$

$$D_1^{-1} R_1^{-1} Q^T K(\mathbf{x}_i, \mathbf{x}_j)^T = [I_{n_i} \quad D_1^{-1} R_1^{-1} R_2 D_2] V^T.$$

Once the above expansion is known, we define the new basis functions as

$$H(\mathbf{x}_i, \mathbf{x}_j) = K(\mathbf{x}_i, \mathbf{x}_j) G.$$

Note that the diagonal elements of $D$ are computed analytically, whereas $R_1^{-1} R_2$ is computed by backward substitution. The relation between the new kernel matrix and the old kernel matrix is given by

$$H(\mathbf{x}_i, \mathbf{x}_j) = K(\mathbf{x}_i, \mathbf{x}_j) G.$$

Instead of solving the original system, $K(\mathbf{x}_i, \mathbf{x}_j) \mathbf{w} = \mathcal{L}^x K(\mathbf{x}_i, \mathbf{x}_i)$, we find $\mathbf{w}$ in the new (discrete) basis via

$$H(\mathbf{x}_i, \mathbf{x}_i) \mathbf{w} = \mathcal{L}^x H(\mathbf{x}_i, \mathbf{x}_i).$$

Note that the right-hand vector can be obtained analytically from (2.20) and (2.21), and that the interpolation matrix with respect to the new kernel, $H(\mathbf{x}_i, \mathbf{x}_i)$, is no longer symmetric.
In practice, some polynomial terms should be added to the expansion (2.14) in order to guarantee polynomial accuracy, or when the kernel $K$ is conditionally positive definite. See (Fasshauer, 2007; Fornberg et al., 2011) for further details.

### 2.5 Numerical Demonstrations

To begin, we consider diffusion on various surfaces $\mathcal{S} \subset \mathbb{R}^2$. Three point local neighbourhoods $X_i$ will be used to extend one layer outwards and one inwards, as shown in Figures 2.1 and 2.2. Throughout this section, we will use the (scaled) Gaussian kernel $K(x, y) = e^{-\frac{1}{2c^2\|x-y\|^2}}$, with various shape parameters $c$, to evaluate the generalized finite difference weights in (2.14) and the power function $P$ in (2.16). The reduced semi-discrete system (2.13) is evolved in time by the forward Euler scheme. As our interest is the spatial discretization of the surface embedding, small time steps are used: $\Delta t = 0.001\hbar^2$ where $\hbar$ is the fill distance (Fasshauer, 2007).

Our first example evolves diffusion on the unit circle. The convergence of the relative errors $\varepsilon$ and the power function $P$ for three different shape parameters, $c = 0.5, 1, 2$ are given in Figure 2.4. Convergence rates are approximately second order for all three tested shape parameters (rates are estimated by the last 5 data points). Notably, the proposed scheme is convergent for all tested shape parameters. Moreover, the power function $P$ also exhibits second order convergence.

To test the performance on nonsmooth curves we apply the same method to a diffusion problem on the square $[-1, 1]^2$. As shown in Figure 2.5, the proposed method is still convergent but the rate drops from second order to first. As in the case of the unit circle, we observe a close agreement between the $\varepsilon$– and $P$–convergence rates. Provided the temporal discretization error is negligible, the numerically accessible convergence rate of $P$ provides a good estimate for the convergence rate of the error. The power function can be
Figure 2.4: Convergence profiles for diffusion on the unit circle $S$. The relative error $\varepsilon$ and power function $P$ are plotted for various grid spacings and shape parameters $c$.

Figure 2.5: Convergence profiles for diffusion on the square $S = [-1, 1]^2$. The relative error $\varepsilon$ and power function $P$ are plotted for various grid spacings and shape parameters $c$. 

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viewed as the local truncation error in the finite difference method.

We emphasize that the evaluation of $P$ is pointwise; that is, at the generalized finite difference stencils (2.9) and (2.14), the power function can be evaluated by the stencils and assigned weights for any SPD kernel, independent of the solution. The value of $P$ yields an upper bound for the spatial discretization error: when the solution is unknown, which is usually the case, the discretization error is bounded by $P$ times an unknown factor $\|u\|_H$. In our convergence plots, we observe that the ratio $\varepsilon/P$ changes with the shape parameter $c$. Since the native space $H$ is generated by the $c$-dependent Gaussian kernel in our demonstrations, different shape parameters yield different spaces $H$ and hence different $\|u\|_H$.

Determining the optimal shape parameter is challenging and is not the purpose of this work. Nonetheless, the introduction of the power function allows an easy way to search for the optimal $c$ by brute force. The values of $P$ shown in Figures 2.4 and 2.5 are the maximum over all stencils used in a particular run. Intuitively, the first order spatial convergence observed in Figure 2.5 is due to the error at the corners (this conjecture can be confirmed numerically). We may determine the optimal shape parameters for a problem with corners by minimizing the power function at the corners. Experimentally, we find $c = 2$ gives good results, so we take it for all computations going forward. Figure 2.6 gives results for diffusion over 3 different folded, triangulated curves. All three cases give similar errors and first order convergence.

The observed quadratic convergence on smooth surfaces and linear convergence on folded surfaces is also found in 3D. In Figure 2.7, the convergence rates (as measured by the max-norm error) for $\varepsilon$ and $P$ are shown for the unit sphere and a punch-in sphere, which is constructed by reflecting all points above $z = 0.5$ in the place $z = 0.5$ (thereby allowing an analytic solution to be derived). For the unit sphere, data points $X$ are quasi-uniformly placed on the manifold (Ling, 2005). For the punch-in sphere we place points along the fold. The local neighborhood of $x_i$ on each smooth (sub-) surface is chosen
Figure 2.6: Convergence profiles for diffusion on various triangles. The relative error $\varepsilon$ and power function $P$ are plotted for various grid spacings with the shape parameter $c = 2.0$. 
Figure 2.7: Convergence profiles for diffusion on the unit sphere $S$ and a punch-in sphere. The relative error $\varepsilon$ and power function $P$ are plotted for various grid spacings and the shape parameter $c = 2.0$. Middle: snapshot of the solution at $t = 1$ for the same initial condition.

to contain 13 points: 5 points are chosen on the fold and 8 on each smooth subsurface. Similar to the treatment in 2D, we average the finite difference weighings over the two subsurfaces to yield the final spatial discretization for points on the fold.

The unit sphere and the punch-in sphere share identical solutions for any given initial condition despite the existence of a fold (we can map between the unit sphere and the punch-in sphere via a reflection in $z = 0.5$). The numerical schemes used for these two manifolds are clearly different and we observe quadratic spatial convergence for the unit sphere and linear convergence for the punch-in sphere. Figure 2.8 shows how the difference between the two numerical schemes evolves over time for one fixed spatial discretization. The top two subfigures are the respective initial conditions: they are identical if we unfold the punch-in sphere. From the snapshots in Figure 2.8, we can see that a disagreement between the two numerical solutions emerges and diffuses away from the fold, which is not surprising since the two numerical recipes are
Initial condition for both unit sphere and punch-in sphere

Figure 2.8: Top: initial conditions. Middle, Bottom: relative difference of the numerical approximation on the unit sphere and the punch-in sphere at various times $t$ with "identical" initial conditions.
different at the fold. We can see that the relative difference grows gradually with time due to the decay of the solution, whereas the absolute difference is rather steady in time. Clearly, the difference is solely due to the treatment of the fold. Note that our initial conditions vary along the meridian lines. This choice was made to avoid over-simplifying the example via symmetric data at the fold.

Not all manifolds are easily unfolded. As an example, consider a flat-top sphere constructed by replacing the $z$-coordinates of the unit sphere by $\min(z, 0.5)$. Figures 2.9 and 2.10 present two simulated results with different initial conditions. The first simulation begins with two hot spots on the large smooth surface symmetric about the $x$-axis. As time evolves, we observe the diffusion progress across the fold to the flat-top and across the large spherical surface. For each snapshot, the maximum and minimum values of the numerical solution are also presented to confirm that the maximum principle is satisfied at consecutive snapshots. The second simulation is initialized with a hot spot located near the edge of the flat-top in order to highlight the method’s treatment of diffusion across a fold. Snapshots are presented at nonuniform times to better visualize the rapid initial flow. We observe that heat flows across the fold at a rate similar to the heat flow within the flat-top. At the final time, the location of hottest temperature coincides with the hot spot for the initial condition. Finally, we note that it will take longer for this simulation to reach steady state due to its more isolated initial profile.

2.6 Reaction-Diffusion system

In this section, we investigate the solution of the system of reaction-diffusion equation. The system of reaction-diffusion equation is given by

$$
\begin{align*}
    u_t &= \nu_u \Delta_S u + f_u(u, v), \\
    v_t &= \nu_v \Delta_S v + f_v(u, v),
\end{align*}
$$

(2.25)
Figure 2.9: Simulation of diffusion on a flat-top sphere with two hot spots in the x-symmetric initial profile.

Figure 2.10: Simulation of diffusion on a flat-top sphere with an off-centered initial hot spot at the top.
subject to the initial condition
\[
\begin{align*}
u(x, 0) &= f(x), \\
v(x, 0) &= g(x).
\end{align*}
\]

### 2.6.1 Brusselator

An particular form of (2.25) which is known as the Brusselator is the model of pattern formation (Turk, 1991; Bertalmio et al., 2001; Ruuth, 1995). Let
\[
\begin{align*}
f_u(u, v) &= a - (b + 1)u + u^2v, \\
f_v(u, v) &= bu - u^2v.
\end{align*}
\]

be the reaction term in (2.25) for Brusselator. Figure 2.11 shows the pattern formation on a surface of cube in \(\mathbb{R}^3\). The parameters are set to be \(a = 3, b = 10.2, \nu = \frac{10}{900}\) for all simulations. The initial condition \(u(x, 0)\) and \(v(x, 0)\) are randomly selected from \([0, 1]^N\).

### 2.6.2 Figzhugh-Nagumo equation

Another special case of reaction-diffusion system will be the Figzhugh-Nagumo equation (FitzHugh, 1961) on surfaces. In this case, the system is
\[
\begin{align*}
\frac{\partial u_S}{\partial t} &= (a - u_S)(u_S - 1)u_S - v_S + \nu \Delta_S u_S \\
\frac{\partial v_S}{\partial t} &= \varepsilon(\beta u_S - v_S)
\end{align*}
\] (2.26)

where \(u_S\) denote the excitation variable. The parameters are set to be \(\varepsilon = 0.01, a = 0.1, \beta = 0.5\) and \(\nu = 0.0001\). Figure 2.12 shows the snapshot of the excitation \(u_S\) at different time \(T\). The spirals are formed as the time evolve. In Figure 2.12, the left column represent a surface of cube in \(\mathbb{R}^3\) while the right column represent a surface of intersection of unit sphere and a annular disk. The homogeneous Neumann boundary condition is imposed to it.
Figure 2.11: Snap Shot of the Brusselator with different diffusive coefficient $D_u$
Figure 2.12: Snap Shot of the excitable media with different time
2.7 Conclusions

We propose an embedding method to solve diffusion on manifolds with folds. Our discretization is based on meshless methods. This approach has the advantage of eliminating the interpolation step in the underlying embedding method, thereby eliminating a source of error and computational cost. Moreover, the flexibility of data point placement is central to our approach for representing folds and the associated differential operators. In future work we will develop extensions of the method to more general operators and more general surfaces. Higher order accurate methods will also be developed.
Chapter 3

$H^2$–Convergence theories for least-squares kernel collocation methods

The strong-form asymmetric kernel-based collocation method, commonly referred to as the Kansa method, is easy to implement and hence is widely used for solving engineering problems and partial differential equations despite the lack of theoretical support. The simple least-squares formulation, on the other hand, makes the study of its solvability and convergence rather nontrivial. In our previous works, we showed how Kansa’s formulation should be modified to guarantee its solvability. We also showed the convergence of an $L^\infty$-minimization formulation, whose solution process requires linear programming solvers. In this paper, we focus on the more welcoming and numerically accessible least-squares approaches. Our analysis is carried out for general second order linear elliptic differential equations in $\Omega \subset \mathbb{R}^d$ under Dirichlet boundary conditions. With kernels that reproduce $H^m(\Omega)$ and some smoothness assumptions on the solution, we provide denseness conditions for a constrained least-squares method and a class of weighted least-squares algorithms to be convergent. Our analysis covers two trial spaces. Theoretically, we identify some $H^2(\Omega)$ convergent LS formulations that have the optimal error estimate
particularly, the proven error bounds identify $d = 2$ as a special case, for which weighted least-squares collocation methods enjoy optimal convergence for a wide range of weights, and this is confirmed numerically. We further verify that the proposed formulations have the optimal $h^m$ convergence rate in $L^2(\Omega)$. We also demonstrate the effects of various collocation settings on the respective convergence rates, as well as how these formulations perform with high order kernels and when coupled with the stable evaluation technique for the Gaussian kernel.

3.1 Introduction

Mathematical models or differential equations are meaningful only if they can somehow mirror the overly complicated real world. Similarly, numerical methods are useful only if they can produce approximations guaranteed to converge to the outcome that the mathematical model predicts. It could take tens of years for some good numerical strategies to mature and become a well-established class of numerical methods with a complete and rigid theoretical framework. Take the finite element method as an example. It waited for a quarter of a century to get its rigorous mathematical foundation. This project aims to continue our theoretical contributions to the unsymmetric radial basis function collocation method, which is also known as the Kansa method in the community and we shall use this name throughout this paper for brevity.

To quickly overview the development of the Kansa method and its connection to the radial basis function (RBF) scattered data interpolation problem, let us look at some of its cornerstones (Fasshauer, 2007; Wendland, 2004; Fasshauer and McCourt, 2015). An RBF is a smooth scalar function $\phi : \mathbb{R}^+ \rightarrow \mathbb{R}$, which usually is induced from a kernel function $\Phi : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ in today’s applications, such that the interpolant of an interpolation problem
is given as a linear combination

\[ u = \sum_{j=1}^{n_Z} \lambda_j \phi(\| \cdot - z_j \|_2) = \sum_{j=1}^{n_Z} \lambda_j \Phi(\cdot, z_j), \quad (3.1) \]

of shifted RBFs in which the set \( Z = \{z_1, \ldots, z_{n_Z} \} \) contains trial centers that specify the shifts of the kernel function in the expansion. Dealing with scaling has been another huge topic in Kansa methods (Golbabai et al., 2015; Kansa and Carlson, 1992; Tsai et al., 2010) for a decade, but we will ignore this point for the sake of simplicity.

Impressed by the meshfree nature, simplicity to program, dimension independence, and arbitrarily high convergence rates interpolations, E.J. Kansa (Kansa, 1990a; Kansa, 1990b) proposed to modify the RBF interpolation method to solve partial differential equations (PDEs) in the early 90s. Using the same RBF expansion (3.1), Kansa imposed strong-form collocation conditions instead of interpolation conditions for identifying the unknown coefficients. Consider a PDE given by \( Lu = f \) in \( \Omega \) and \( Bu = g \) on \( \Gamma = \partial \Omega \). The Kansa method collocates the PDE at the trial centers \( Z \) to yield exactly \( n_Z \) conditions:

\[ Lu(z_i) = \sum \lambda_j L\phi(\| z_i - z_j \|), \quad \text{for} \quad z_i \in Z \cap \Omega, \]
\[ Bu(z_i) = \sum \lambda_j B\phi(\| z_i - z_j \|), \quad \text{for} \quad z_i \in Z \cap \Gamma, \]

for identifying the unknown \( \lambda_j \) or equivalently, a numerical approximation to \( u \) from the trial space

\[ U_Z = U_{Z,\Omega,\Phi} := \text{span}\{ \Phi(\cdot - z_j) : z_j \in Z \}. \quad (3.3) \]

This approach requires no re-formulation of the PDE and no triangulation. As long as one knows how to program for an interpolation problem, it only takes minutes to understand and code up something for the Kansa method. Since invented, the Kansa method has been widely used in vast numbers of applications in physics and engineering (Chen et al., 2011; Kansa and Geiser, 2013; Li et al., 2015; Pang et al., 2015).
Since the differential and boundary operators of a PDE are independently applied to yield different rows of the final linear system of equations, it is easy to see why any Kansa system matrix is unsymmetric. While this has some implications for the choice of linear solvers, the unsymmetric matrix places the Kansa method far away from the approximation theories from which RBFs interpolation theories were built. Though the technique introduced by Kansa is very successful in a large variety of applications in Engineering and Science, there were no proven results about it for over 10 years. After many unsuccessful attempts to establish such a foundation, Hon and Schaback (Hon and Schaback, 2001) showed in 2001 that there are extremely rare cases where the original approach can fail because the underlying linear system can be singular. This put an end to all attempts to prove stability of the Kansa method in general. One workaround is to apply symmetric collocation (Fasshauer, 1999; Franke and Schaback, 1998) that mimics scattered Hermite interpolation. While the Kansa trial space basis in (3.1) is independent of the collocation, the symmetric method takes a basis that is itself dependent on the collocation. This approach yields positive definite symmetric system matrices at the expense of higher smoothness requirements and less stability. On the positive side, symmetric collocation can be proven (Schaback, 2015) to be error-optimal, because it is a pointwise optimal recovery of the solution from discrete input data.

The situation for the Kansa method remained the same until 2006, when we provided the first solvability results for an extended Kansa method. In order to ensure solvability, overtesting is applied. Keeping the trial space (3.3) based on a set $Z$ of trial centers, the standard Kansa system (3.2) is modified by taking another, but usually larger discrete set $X$ of collocation points that is sufficiently fine relative to the set $Z$ of trial centers. Readers are referred to the original articles (Ling et al., 2006) and an extension (Schaback, 2007) to the corresponding weak problems for details. In 2008, we had a partial answer to the convergence of an overdetermined Kansa formulation (Ling and Schaback, 2008). Our analysis was carried out based on the continuous and discrete
maximum norms. We showed that the \( \ell^\infty \)-minimizer of a residual functional converges to the exact solution at the optimal speed, i.e. with the same convergence rate as the interpolant converges to the exact solution. From then on, we attempted to extend the theories to the least-squares (LS) minimizer (Kwok and Ling, 2009) and numerically verified in extended precision arithmetic that the LS-minimizer also converges at the optimal rate (Lee et al., 2009). In this study, we reexamine the overdetermined Kansa method and concentrate on the popular LS solution. In Section 3.2, we will provide all the necessary assumptions and prove error estimates for a constrained least-squares (CLS) and a class of weighted least-squares (WLS) formulations. The convergence for the CLS formulation will then be given in Section 3.3. In Section 3.4 and 3.5, the theory for WLS formulations in two trial spaces will be given. Lastly, we will numerically verify the accuracy and convergence rates of some proven convergent formulations in Section 3.6.

3.2 Notations, assumptions and main theorems

Throughout the paper, the notation \( C \) will be reserved for generic constants whose subscripts indicate the dependencies of the constant.

We consider a general second order elliptic differential equation in some domain \( \Omega \subset \mathbb{R}^d \) subject to the Dirichlet boundary condition on \( \Gamma = \partial \Omega \):

\[
\mathcal{L} u = f \quad \text{in } \Omega, \\
u = g \quad \text{on } \Gamma.
\] (3.4)

The differential operator is

\[
\mathcal{L} u := \sum_{i,j=1}^{d} \frac{\partial}{\partial x^j} \left( a^{ij}(x) \frac{\partial}{\partial x^i} u(x) \right) + \sum_{j=1}^{d} \frac{\partial}{\partial x^j} \left( b^j(x) u(x) \right) \\
+ \sum_{i=1}^{d} c^i(x) \frac{\partial}{\partial x^i} u(x) + d(x) u(x) = f(x).
\] (3.5)

The Sobolev regularity of the true solution will be denoted by \( m \), and we will work with standard Hilbert spaces \( H^k(\Omega) \) and \( H^{k-1/2}(\Gamma) \) with norms \( \|u\|_{k,\Omega} \) and \( \|u\|_{k-1/2,\Gamma} \), respectively, for \( k \leq m \).
**Assumption 5** (Smoothness of domain and solution). We assume that the bounded domain $\Omega$ has a piecewise $C^m$-boundary $\Gamma$ so that $\Omega$ is Lipschitz continuous and satisfies an interior cone condition. Also, we assume that the functions $f$ and $g$ are smooth enough to admit a classical solution $u^* \in H^m(\Omega)$. □

Now the trace theorem (Wloka, ) can be applied and we can define a trace operator:

$$\mathcal{T} : H^m(\Omega) \to H^{m-1/2}(\Gamma)$$

such that $\mathcal{T} u = u|_{\Gamma}$ for all $u \in C^m(\bar{\Omega})$, for $m > 1/2$, with a continuous right-inverse linear extension operator $\mathcal{E}$ such that

$$\mathcal{T} \circ \mathcal{E} g = g$$

for all $g \in H^{m-1/2}(\Gamma)$.

The smoothness assumption also allows a partition of unity of the boundary, each part of which can be mapped to the unit ball in $\mathbb{R}^{d-1}$ by a $C^m$–diffeomorphism. This allows us to define Sobolev norms on $\Gamma$ and apply some Sobolev inequalities (i.e., kernel independent ones).

Let $\chi$ be any discrete set of $n_\chi$ points in $\Omega$. For any $u \in H^m(\Omega)$ we define discrete norms on $\chi$ by

$$\|u\|_\chi = \|u\|_{0,\chi} = \|u\|_{L^2(\chi)}, \quad \|u\|_{k,\chi} := \left( \sum_{|\alpha| \leq k} \|D^\alpha u\|_\chi^2 \right)^{1/2}, \quad 0 \leq k < m - d/2,$$

where $\alpha$ is some multi-index and $D^\alpha u \in C(\Omega)$ are weak derivatives of $u$. The same notations will also be used to denote discrete norms on boundary for any discrete set $\chi \subset \Gamma$.

**Assumption 6** (Differential operator). Let $m > 3 + d/2$. Assume that $\mathcal{L}$ as in (3.5) is a strongly elliptic operator with coefficients belonging to $W^{m}_\infty(\Omega)$. □

Then, by results in (Giesl and Wendland, 2007), $\mathcal{L}$ is a bounded operator from $H^m(\Omega)$ to $H^{m-2}(\Omega)$ with

$$\|\mathcal{L} u\|_{m-k,2,\Omega} \leq C_{\Omega,\mathcal{L}} \|u\|_{m-k,\Omega}, \quad 2 \leq k \leq m - 2,$$

(3.6)
for all $u \in H^m(\Omega)$. Also by the boundedness of the derivatives of the coefficients, we can easily get a discrete analog for any discrete set $\chi \subset \Omega$,

$$\|Lu\|_{m-k-2,\chi} \leq C_{\Omega,L}\|u\|_{m-k,\chi}, \quad d/2 < k \leq m - 2. \quad (3.7)$$

Moreover, the following boundary regularity estimate (Jost, 2007) holds:

$$\|u\|_{k+2,\Omega} \leq C_{\Omega,L,k} \left( \|Lu\|_{k,\Omega} + \|u\|_{k+1+1/2,\Gamma} \right), \quad 0 \leq k \leq m - 2, \quad (3.8)$$

for all $u \in H^m(\Omega)$ with $C_{\Omega,L,k}$ depending on $\Omega$, the ellipticity constant of $L$, and $k \geq 0$.

**Assumption 7** (Kernel). Assume $\Phi$ is a reproducing kernel of $H^m(\Omega)$ for some integer $m > 2 + d/2$ and $m \geq 4$. More precisely, we use a symmetric positive definite kernel $\Phi$ on $\mathbb{R}^d$ with smoothness $m$ that satisfies

$$c_{\Phi,m} (1 + \|\omega\|^2_2)^{-m} \leq \hat{\Phi}_m(\omega) \leq C_{\Phi,m} (1 + \|\omega\|^2_2)^{-m} \quad \text{for all } \omega \in \mathbb{R}^d, \quad (3.9)$$

for two constants $0 < c_{\Phi,m} \leq C_{\Phi,m}$. \hfill \Box

For any $m > d/2$, its native space $\mathcal{N}_{\Omega,\Phi}$ on $\mathbb{R}^d$ (Buhmann, 2003; Wendland, 2004) is norm-equivalent to $H^m(\mathbb{R}^d)$. The standard Whittle-Matérn-Sobolev kernel with exact Fourier transform $(1 + \|\omega\|^2_2)^{-m}$ takes the form

$$\Phi(x) := \|x\|^{m-d/2}_2 K_{m-d/2}(\|x\|_2) \quad \text{for all } x \in \mathbb{R}^d,$$

where $K_{\nu}$ is the Bessel functions of the second kind. The compactly supported piecewise polynomial Wendland functions (Wendland, 1998) are another examples of kernels satisfying (3.9).

**Assumption 8** (Trial space). Let $Z = \{z_1, \ldots, z_{nz}\}$ be a discrete set of trial centers in $\Omega$. In analogy to (3.3), but now with translation-invariance, we define the finite-dimensional trial space $\mathcal{U}_Z$ as

$$\mathcal{U}_Z = \mathcal{U}_{Z,\Omega,\Phi} := \text{span}\{\Phi(\cdot - z_j) : z_j \in Z\} \subset \mathcal{N}_{\Omega,\Phi}.$$

\hfill \Box
For describing the denseness of \( Z \subset \Omega \), its *fill distance* for fixed \( \Omega \) and separation distance are defined as
\[
q_Z := \frac{1}{2} \min_{z_i \neq z_j} \| z_i - z_j \|_{\ell_2(\mathbb{R}^d)},
\]
respectively, and the quantity \( h_Z / q_Z =: \rho_Z \) is commonly referred as the *mesh ratio* of \( Z \). For any \( u \) in the native space \( \mathcal{N}_{\Omega, \Phi} \) of \( \Phi \), we denote \( I_Z u \) to be the interpolant of \( u \) on \( Z \) from the trial space \( U_Z \).

**Assumption 9 (Collocation points).** Let \( X = \{ x_1, \ldots, x_{n_X} \} \) be a discrete set of PDE collocation points in \( \Omega \) and \( Y = \{ y_1, \ldots, y_{n_Y} \} \) be a set of boundary collocation points on \( \Gamma \). We assume the set \( Z \) of discrete trial centers to be sufficiently dense and the sets of points \( X \) and \( Z \) to be asymptotically quasi-uniform. That is, there exist constants \( \gamma_\chi > 1 \) such that
\[
\gamma_\chi^{-1} q_\chi \leq h_\chi \leq \gamma_\chi q_\chi. \quad \text{for } \chi \in \{ X, Z \}. \tag{3.10}
\]
We further assume that the two sets \( X \) and \( Y \) of collocation points are as fine as \( Z \) in the sense that the relative fill distances \( h_X / h_Z \) and \( h_Y / h_Z \) are sufficiently small with respect to \( \Omega, \Phi, \) and \( \mathcal{L} \) but independent of the solution \( u^* \). \( \square \)

Note that the sets \( X \) and \( Y \) of collocation points together have to be as dense as the trial centers in \( Z \) to ensure stability.

Imposing strong testing on (3.4) at collocation points in \( X \) and \( Y \) yields \( n_X + n_Y > n_Z \) conditions, from which one can hopefully identify a numerical approximation from some trial spaces. The following theorems summarize our convergence results for three possible least-squares alternatives. The first concerns the case where we enlarge the set \( Z \) of trial points by adding the set \( Y \) of boundary collocation points to it. Then we can keep the numerical solution to be exact on \( Y \), and we add this as a constraint.

**Theorem 10 (Constrained least squares (CLS)).** Suppose the Assumptions 5 to 9 hold. Let \( u^* \in H^m(\Omega) \) denote the exact solution of the elliptic PDE (3.4) and let \( u_{X,Y}^{CLS} \in U_{Z,Y} \) be the constrained least-squares solution defined as
\[
u_{X,Y}^{CLS} := \arg \inf_{u \in U_{Z,Y}} \| \mathcal{L} u - f \|_X^2 \quad \text{subject to } u_{|Y} = g_{|Y}. \tag{3.11}
\]
Then the error estimate
\[ \| u_{X,Y}^{CLS} - u^* \|_{2,\Omega} \leq C_{\Omega,\Phi,\mathcal{L},\gamma_X} h_{Z,Y}^{m-2} \| u^* \|_{m,\Omega}, \]
holds for some constant \( C_{\Omega,\Phi,\mathcal{L},\gamma_X} \) that depends only on \( \Omega, \Phi, \mathcal{L}, \) and the uniformity constant \( \gamma_X \) of \( X \).

The next case does not require exactness on \( Y \) but still keeps \( Z \cap Y \) as the set of trial centers.

**Theorem 11 (Weighted least squares (WLS)).** Suppose the Assumptions 5 to 9 hold. Let \( u^* \in H^m(\Omega) \) denote the exact solution of the elliptic PDE (3.4) and let \( u_{X,Y,Z,Y}^{\text{WLS},\theta} \in \mathcal{U}_{Z,Y} \) be the weighted least-squares solution defined as
\[
u_{X,Y,Z,Y}^{\text{WLS},\theta} := \arg \inf_{u \in \mathcal{U}_{Z,Y}} \| \mathcal{L} u - f \|_X^2 + \left( \frac{h_Y}{h_X} \right)^{\theta/2} h_Y^{-2\theta} \| u - g \|_Y^2, \quad 0 \leq \theta. \tag{3.12} \]
Then, with \( h_X \leq h_Y < 1 \),
\[
u_{X,Y,Z,Y}^{\text{WLS},\theta} - u^* \|_{2,\Omega} \leq C_{\Omega,\Phi,\mathcal{L},\gamma_X} \left( 1 + h_x^{(d-2)/4} h_Y^{(d-2)(d-4)/4} \right) h_{Z,Y}^{m-2} \| u^* \|_{m,\Omega}, \]
for \( 0 \leq \theta \leq 2 \), and
\[
u_{X,Y,Z,Y}^{\text{WLS},\theta} - u^* \|_{2,\Omega} \leq C_{\Omega,\Phi,\mathcal{L},\gamma_X} h_{Z,Y}^{m-2} \| u^* \|_{H^m(\Omega)}, \]
for \( 2 \leq \theta \leq \infty \), hold for some constant \( C_{\Omega,\Phi,\mathcal{L}} \) that depends only on \( \Omega, \Phi, \) and \( \mathcal{L} \).

Finally, we go back to the case where \( Z \) is the set of trial nodes, independent of \( X \) and \( Y \).

**Theorem 12 (WLS in a smaller trial space).** Suppose the trial space of the weighted least-squares approximation in Theorem 11 is restricted to \( u_{X,Y,Z}^{\text{WLS},\theta} \in \mathcal{U}_Z \) instead of \( \mathcal{U}_{Z,Y} \). Further assume that the sets \( Y \) are asymptotically quasi-uniform with constant \( \gamma_Y > 1 \) as in (3.10) and \( h_Y \leq h_Z \). Then, the error estimate becomes
\[
u_{X,Y,Z}^{\text{WLS},\theta} - u^* \|_{2,\Omega} \leq C_{\Omega,\Phi,\mathcal{L},\gamma_Y} \left( 1 + h_x^{(d-2)/4} h_Y^{(d-2)(d-4)/4} + h_Y^2 h_Z^2 \right) h_{Z,Y}^{m-2} \| u^* \|_{m,\Omega}, \]
for any \( 0 \leq \theta \leq 2 \), and some constant \( C_{\Omega,\Phi,\mathcal{L},\gamma_Y} \) that depends only on \( \Omega, \Phi, \mathcal{L}, \) and uniformity constants \( \gamma = [\gamma_X, \gamma_Y, \gamma_Z] \).
3.3 Optimal convergence for CLS

We first prove some necessary inequalities essential to our proofs.

**Lemma 13** (Sampling Inequality of fractional order). Suppose $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain with a piecewise $C^m$–boundary. Then, there exists a positive constant $C_{\Omega,m,s}$ depending on $\Omega$, $m$ and $s$ such that the following holds:

$$\|u\|_{s,\Omega} \leq C_{\Omega,m,s} \left( h_X^{m-s} \|u\|_{m,\Omega} + h_X^{d/2-s} \|u\|_{X} \right), \quad 0 \leq s \leq m,$$

and

$$\|u\|_{s-1/2,\Gamma} \leq C_{\Omega,m,s} \left( h_Y^{m-s} \|u\|_{m,\Omega} + h_Y^{d/2-s} \|u\|_{Y} \right), \quad 1/2 \leq s \leq m,$$

for any $u \in H^m(\Omega)$ with $m > d/2$ and any discrete sets $X \subset \Omega$ and $Y \subset \Gamma$ with sufficiently small mesh norm $h_X$ and $h_Y$.

**Proof.** The interior sampling inequality for $X \subset \Omega$, which only requires $\Omega$ be a bounded Lipschitz domain, is a special case of a sampling inequality in (Arcangeli et al., 2012). Applying the interior sampling inequality to the union of unit balls in $\mathbb{R}^{d-1}$, which are images of the partition of unity of $\Gamma$ under the $C^m$–diffeomorphism in Assumption 5, yields

$$\|u\|_{s-1/2,\Gamma} \leq C \left( h_Y^{(m-1/2) - (s-1/2)} \|u\|_{m-1/2,\Gamma} + h_Y^{(d-1)/2 - (s-1/2)} \|u\|_{Y} \right),$$

for all $1/2 \leq s \leq m$. Finally, by applying the trace theorem, the desired boundary sampling inequality is obtained. \qed

**Lemma 14** (Interpolation estimate). Let a kernel $\Phi$ as in (3.9) with smoothness $m$ be given. Suppose $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain satisfying an interior cone condition. Let $Z \subset \Omega$ be a discrete set of trial centers with mesh norm $h_Z < m^{-2} C_{\Omega}$ for some constant $C_{\Omega}$ depending only on $\Omega$. Let $X \subset \Omega$ be another discrete set with $h_X \leq h_Z$. If $f \in H^m(\Omega)$, then its interpolant $I_Z f$ on $Z$ from $U_Z$ is a good approximation to the least-squares fit in the sense that

$$\|f - I_Z f\|_{k,X} \leq C_{\Omega,\Phi,k} n_X^{1/2} \rho_X^{d/2} h_Z^{m-k} \|f\|_{m,\Omega}, \quad 0 \leq k < m - 1 - d/2,$$

for some constant $C_{\Omega,\Phi,k}$, depending only on $\Omega$, $k$, and $\Phi$. 

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Proof. Applying (Narcowich et al., 2005, Prop.3.3) to our Hilbert space setting and taking care of the definitions of discrete norms yield the desired LS error bound. □

Lemma 15 (Inverse Inequality). Let a kernel $\Phi_m : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ satisfying (3.9) with smoothness $m$ be given. Suppose $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain satisfying an interior cone condition. Assume $0 \leq \nu \leq m - d/2$ and $d/2 < \sigma \leq m - 2\nu$ for some integers $\nu$ and positive $\sigma$. Then there is a constant $C_{\Omega, \Phi_m, \sigma, \nu}$, depending only on $\Omega, \Phi_m, \sigma$, and $\nu$ such that

$$\|u\|_{\sigma + 2\nu, \Omega} \leq C_{\Omega, \Phi_m, \sigma, \nu} \rho_Z^{m - \nu} h_Z^{-\sigma} \|u\|_{2\nu, \Omega}$$

(3.13) holds for all $u \in U_Z$ from the trial space of $\Phi_m$ on all sufficiently dense and quasi-uniform sets $Z \subset \Omega$ with fill distance $h_Z$ and mesh ratio $\rho_Z$.

Proof. The basic proof idea is to use an inverse inequality from (Hangelbroek et al., 2015, Eqn. 3.19). It has the $L_2(\Omega)$ norm on the right-hand side, but for (3.13) we have to go over to derivatives there. The idea is to push the derivatives into a new kernel.

Let $\Phi_m$ denote the given kernel satisfying (3.9) with parameter $m$. For all $0 \leq \nu < m - d/2$, we define symmetric positive definite kernels $\Psi_{m - \nu} := (I - \Delta)^{\nu/2} \Phi_m$, whose Fourier transforms satisfy

$$c_1 (1 + \|\omega\|^2)^{-(m - \nu)} \leq \hat{\Psi}_{m - \nu}(\omega) = (1 + \|\omega\|^2)^{\nu} \hat{\Phi}_m(\omega) \leq C_1 (1 + \|\omega\|^2)^{-(m - \nu)},$$

and hence, $\Psi_{m - \nu}$ has behavior like $\Phi_{m - \nu}$. This is like applying the operator $(1 - \Delta)^{\nu/2}$ to both arguments of $\Phi_m$, if $\Phi_m$ is written in difference form.

We use the notation $u_{\beta, Z, \Phi_m} := \sum_{j \in Z} \beta_j \Phi_m(\cdot - z_j)$ to denote the functions in the trial space $U_{Z, \Phi_m}$ spanned by translates of the kernel $\Phi_m$ on the trial centers in $Z$ with coefficients forming a vector $\beta \in \mathbb{R}^{|Z|}$. Then

$$(I - \Delta)^{\nu} u_{\beta, Z, \Phi_m} = u_{\beta, Z, \Psi_{m - \nu}}$$

holds, and these are the functions that we use in (Hangelbroek et al., 2015, Eqn. 3.19). This yields

$$\|u_{\beta, Z, \Psi_{m - \nu}}\|_{\sigma, \Omega} \leq C_{\Omega, \Phi_m, \sigma, \nu} \rho_Z^{m - \nu} h_Z^{-\sigma} \|u_{\beta, Z, \Psi_{m - \nu}}\|_{0, \Omega}.$$
for all \( \beta \in \mathbb{R}^{|Z|} \) and \( 0 \leq \nu < m - d/2, \ 0 \leq \sigma \leq m - \nu \). The right hand side is what we want, because of

\[
\| u_{\beta,Z,\Psi_{m-\nu}} \|_{0,\Omega}^2 = \int_{\Omega} |(I - \Delta)^\nu u_{\beta,Z,\Phi_m} |^2 \, dx \\
\leq C_{\Omega,\nu} \sum_{|\alpha| \leq 2\nu} \int_{\Omega} |D^\alpha u_{\beta,Z,\Phi_m} |^2 \, dx \\
= C_{\Omega,\nu} \| u_{\beta,Z,\Phi_m} \|_{2\nu,\Omega}^2,
\]

for \( 2\nu \leq m \). We are now left with

\[
\| u_{\beta,Z,\Psi_{m-\nu}} \|_{\sigma,\Omega}^2 = \|(I - \Delta)^\nu u_{\beta,Z,\Phi_m} \|_{\sigma,\Omega}^2
\]

and our goal is to bound this from below by \( \| u_{\beta,Z,\Phi_m} \|_{2\nu+2\nu,\Omega}^2 \). By definition via Fourier transforms,

\[
H^k_2(\mathbb{R}^d) = \{ v : (1 + \| \omega \|_2^2)^{k/2} \hat{v}(\omega) \in L^2(\mathbb{R}^d) \}.
\]

We use the sloppy notation \( \Phi_k \) to denote kernels in the family of \( \Phi_m \) with smoothness \( d/2 < k \leq m \). Then, \( H^k_2(\mathbb{R}^d) \) is norm equivalent to the native space \( N_{\Phi_k}(\mathbb{R}^d) \) of \( \Phi_k \) on \( \mathbb{R}^d \) and equal as sets; i.e.,

\[
c_{\Phi_m,k} \| u \|_{N_{\Phi_k}(\mathbb{R}^d)} \leq \| u \|_{H^k_2(\mathbb{R}^d)} \leq C_{\Phi_m,k} \| u \|_{N_{\Phi_k}(\mathbb{R}^d)}
\]

for some constants \( 0 < c_{\Phi_m,k} \leq C_{\Phi_m,k} \). Before we go over to subdomains, we note that the Fourier transform of the operator \( I - \Delta \) is \( 1 + \| \omega \|_2^2 \), and this extends to arbitrary non-integer powers. Thus,

\[
(I - \Delta)^\nu H^k_2(\mathbb{R}^d) = H^{k+2\nu}_2(\mathbb{R}^d), \ 0 \leq 2\nu \leq m - k,
\]

and

\[
\| (I - \Delta)^\nu u \|_{H^k_2(\mathbb{R}^d)} = \| u \|_{H^{k+2\nu}_2(\mathbb{R}^d)} \text{ for all } u \in H^{k+2\nu}_2(\mathbb{R}^d), \ 0 \leq 2\nu \leq m - k.
\]

For a domain \( \Omega \subset \mathbb{R}^d \) with Lipschitz boundary, we also have that \( N_{\Phi_k}(\Omega) \) and \( H^k_2(\Omega) \) are equal as sets and the norms are equivalent (Wendland, 2004, Cor 10.48), where \( H^k_2(\Omega) \) has the standard definition via weak derivatives and
$N_{\Phi_k}(\Omega)$ has the standard definition via a closure of $\Phi_k$-translates. We use the sloppy notation

$$c_{\Omega, \Phi_m, k} \|u\|_{N_{\Phi_k}(\Omega)} \leq \|u\|_{H_k^2(\Omega)} \leq C_{\Omega, \Phi_m, k} \|u\|_{N_{\Phi_k}(\Omega)}$$

for some constants $0 < c_{\Omega, \Phi_m, k} \leq C_{\Omega, \Phi_m, k}$. By Theorem 10.47 there, the restriction operator $R_{\Phi_k, \Omega} : N_{\Phi_k}(\mathbb{R}^d) \rightarrow N_{\Phi_k}(\Omega)$ is well-defined and satisfies

$$\|R_{\Phi_k, \Omega}v\|_{N_{\Phi_k}(\Omega)} \leq \|v\|_{N_{\Phi_k}(\mathbb{R}^d)}$$

for all $v \in N_{\Phi_k}(\mathbb{R}^d)$.

Going the other way, there is an isometric extension operator $E_{\Phi_k, \Omega} : N_{\Phi_k}(\mathbb{R}^d) \rightarrow N_{\Phi_k}(\mathbb{R}^d)$ (Wendland, 2004, Th. 10.46). Most of this can already be found in (Schaback, 1997). Another extension operator is $E_k, \Omega : H^2_k(\Omega) \rightarrow H^2_k(\mathbb{R}^d)$, and it is bounded. This takes into account that the global space is defined via Fourier transforms, while the local one has $L_2$ integrals over weak derivatives.

It is known that the Sobolev extension operators do not commute with general derivatives. On the trial functions, we do have $E_{\Phi_m, \sigma}(I - \Delta)^{\nu} = (I - \Delta)^{\nu} E_{\Phi_m, \sigma + 2\nu}$ for $m - \nu > d/2$ and $0 \leq \sigma + 2\nu \leq m$ since

$$E_{\Phi_m, \sigma}(I - \Delta)^{\nu} u_{\beta, Z, \Phi_m} = E_{\Phi_m, \sigma}(I - \Delta)^{\nu} u_{\beta, Z, \Phi_m} = (I - \Delta)^{\nu} u_{\beta, Z, \Phi_m} = (I - \Delta)^{\nu} E_{\Phi_m, \sigma + 2\nu}(I - \Delta)^{\nu} u_{\beta, Z, \Phi_m}$$

(3.14)

hold if the functions lie in the correct space, i.e.,

$$E_{\Phi_m, \sigma} u_{\beta, Z, \Phi_m} = u_{\beta, Z, \Phi_m}, \quad \text{and} \quad E_{\Phi_m, \sigma + 2\nu} u_{\beta, Z, \Phi_m} = u_{\beta, Z, \Phi_m}.$$

The functions are globally defined anyway, and thus they coincide with their extension if the global norms are bounded. Thus, we need that

$$u_{\beta, Z, \Phi_m} \in N_{\Phi_m}(\mathbb{R}^d), \quad \text{and} \quad u_{\beta, Z, \Phi_m} \in N_{\Phi_m+2\nu}(\mathbb{R}^d).$$

The condition for the first case is $2(m - \nu) - \sigma > d/2$. The second case requires a finite $d$-variate integral over

$$|\hat{\Phi}_m(\omega)|^2 (1 + \|\omega\|^2_2)^{\sigma + 2\nu} = (1 + \|\omega\|^2_2)^{-2m + \sigma + 2\nu},$$
that yields the same condition. Using the native space extension operators, we get

\[
\| (I - \Delta)^\nu u_{\beta,Z,\Phi_m} \|_{H^2_\sigma(\Omega)} \geq C_{\Omega,\Phi_m}\| (I - \Delta)^\nu u_{\beta,Z,\Phi_m} \|_{N_{\Phi_m}(\Omega)}
\]

\[
= C_{\Omega,\Phi_m}\| E_{\Phi_m}\Omega (I - \Delta)^\nu u_{\beta,Z,\Phi_m} \|_{N_{\Phi_m}(\mathbb{R}^d)}
\]

\[
\geq C'_{\Omega,\Phi_m}\| E_{\Phi_m}\Omega (I - \Delta)^\nu u_{\beta,Z,\Phi_m} \|_{H^2_\sigma(\mathbb{R}^d)},
\]

and, by the extension identity (3.14),

\[
\| (I - \Delta)^\nu u_{\beta,Z,\Phi_m} \|_{H^2_\sigma(\Omega)} \geq C'_{\Omega,\Phi_m}\| (I - \Delta)^\nu E_{\Phi_m+2\nu}\Omega u_{\beta,Z,\Phi_m} \|_{H^2_\sigma(\mathbb{R}^d)}
\]

\[
= C'_{\Omega,\Phi_m}\| E_{\Phi_m+2\nu}\Omega u_{\beta,Z,\Phi_m} \|_{H^2_\sigma(\mathbb{R}^d)}.
\]

We now go local by

\[
\| (I - \Delta)^\nu u_{\beta,Z,\Phi_m} \|_{H^2_\sigma(\Omega)} \geq C'_{\Omega,\Phi_m}\| E_{\Phi_m+2\nu}\Omega u_{\beta,Z,\Phi_m} \|_{N_{\Phi_m+2\nu}(\Omega)}
\]

\[
= C'_{\Omega,\Phi_m}\| u_{\beta,Z,\Phi_m} \|_{N_{\Phi_m+2\nu}(\Omega)}
\]

\[
\geq C''_{\Omega,\Phi_m}\| u_{\beta,Z,\Phi_m} \|_{H^2_\sigma(\mathbb{R}^d)}.
\]

We completed proving a local Bernstein inequality; note that the weaker norm on the right hand side must take an even order, whereas the global counterpart (Narcowich et al., 2006) allows any nonnegative integer orders. □

**Lemma 16 (H^2–Stability).** Let a kernel \( \Phi \) as in (3.9) with smoothness \( m \geq 4 \) be given. Suppose \( \Omega \subset \mathbb{R}^d \) is a bounded Lipschitz domain satisfying an interior cone condition. If the elliptic operator \( \mathcal{L} \) satisfies all assumptions to allow regularity (3.8), then there exists a constant \( C_{\Omega,\mathcal{L}} \), depending only on \( \Omega, \Phi, \) and \( \mathcal{L} \) such that

\[
\| u \|_{2,\Omega} \leq C_{\Omega,\mathcal{L}} \left( h_{X}^{d/2} \| \mathcal{L} u \|_{X} + h_{Y}^{d/2-2} \| u \|_{Y} \right)
\]

holds for all \( u \in U_{Z,Y} \) in the trial space of \( \Phi \) on \( Z \cup Y \) for any sufficiently dense and quasi-uniform sets \( Z \subset \Omega \), and any finite sets \( X \subset \Omega \) and \( Y \subset \Gamma \) with sufficiently small relative fill distances \( h_{X}/h_{Z} \) and \( h_{Y}/h_{Z} \).

Note that the factor at the second term is not \( h_{Y}^{(d-1)/2} \) as one would expect. This might be connected to the fact that the natural norm on the boundary is the \( L_{\infty} \) norm, due to the Maximum Principle.
Proof. We start by applying the sampling inequality of Lemma 13 (or the original one proposed in (Madych, 1992)) to the function $\mathcal{L}u \in H^m(\Omega)$ and get
\[
\|\mathcal{L}u\|_{0,\Omega} \leq C_\Omega(h_X \|\mathcal{L}u\|_{1,\Omega} + h_X^{d/2} \|\mathcal{L}u\|_{0,X}).
\]
Applying (3.6) to remove $\mathcal{L}$ from the first term on the right, we have
\[
\|\mathcal{L}u\|_{0,\Omega} \leq C_\Omega(h_X \|u\|_{3,\Omega} + h_X^{d/2} \|\mathcal{L}u\|_{0,X}). \tag{3.15}
\]
Similarly, we can sample $u$ at the boundary points in $Y$ by Lemma 13 so that
\[
\|u\|_{1+1/2,\Gamma} \leq C_\Omega(h_Y \|u\|_{3,\Omega} + h_Y^{d/2} \|u\|_{Y}). \tag{3.16}
\]
Putting (3.15) and (3.16) into the $H^2$ regularity estimate (3.8):
\[
\|u\|_{2,\Omega} \leq C_\Omega,\mathcal{L} (\|\mathcal{L}u\|_{0,\Omega} + \|u\|_{1+1/2,\Gamma}),
\]
we obtain
\[
\|u\|_{2,\Omega} \leq C_\Omega,\mathcal{L} (h_X^{d/2} \|\mathcal{L}u\|_{0,X} + h_Y^{d/2} \|u\|_{Y} + (h_X^{m-2} + h_Y^{m-2}) \|u\|_{m,\Omega}). \tag{3.17}
\]
Equation (3.17) is now reduced to the following inequality with $\|u\|_{2,\Omega}$ on both sides:
\[
\|u\|_{2,\Omega} \leq C_\Omega,\mathcal{L} (h_X^{d/2} \|\mathcal{L}u\|_{0,X} + h_Y^{d/2} \|u\|_{Y}) + C_\Omega,\mathcal{L} (h_X^{m-2} + h_Y^{m-2}) h_Y^{-m+2} \|u\|_{2,\Omega}.
\]
Assume all sets are dense enough so fill distances are correctly measured. By using $Z$ away from boundary points $Y$ by distance $h_Y$, $Y$ and $Z$ being quasi-uniform, and $h_X \approx h_Y$. Then, $h_{Z\cup Y} \approx h_Z$ and $q_{Z\cup Y} \approx q_Y \approx h_Y$ The dense requirement reads like $C_\Omega,\mathcal{L} (h_Y/h_Z + (h_X/h_Y)^{m-2}h_Y/h_Z) < 1/2$ and is achievable by $h_X, h_Y < h_Z$ but in the same order.

Therefore, for small enough relative fill distance, i.e.,
\[
C_\Omega,\mathcal{L} (h_Y/h_Z + (h_X/h_Y)^{m-2}h_Y/h_Z) < 1/2, \tag{3.18}
\]
the desired stability result follows. \qed
Lemma 17 (Consistency). If the elliptic operator $L$ satisfies all assumptions to allow (3.7), and with the assumptions of Lemma 14, we have

$$\min_{v \in \mathcal{U}_{Z \cup Y}} \|Lv - Lu^*\|_X \leq C_{\Omega, \Phi, L} h_X^{1/2} \rho_X^{d/2} h_{Z \cup Y}^{m-2}\|u^*\|_{m, \Omega},$$

for any $u^* \in H_0^m(\Omega)$.

**Proof.** We compare the minimizer $v^* \in \mathcal{U}_{Z \cup Y}$ of the optimization problem with the interpolant $I_{Z \cup Y}u^* \in \mathcal{U}_{Z \cup Y}$ that also has zeros at $Y$ because $u^* \in H_0^m(\Omega)$ does. Therefore, by (3.7),

$$\|Lv^* - Lu^*\|_X \leq \|LI_{Z \cup Y}u^* - Lu^*\|_X \leq C_{\Omega, L}\|I_{Z \cup Y}u^* - u^*\|_{2, X}.$$  

Consistency of the CLS formulation in (3.11) follows immediately after applying an interpolation estimate (Lemma 14).

To prove Theorem 10, suppose Assumptions 5–9 hold so that all lemmas in this section can be applied.

### 3.3.1 Homogenous boundary

To begin, we consider the PDE (3.4) with homogenous boundary condition:

$$Lw = f \text{ in } \Omega, \quad w|\Gamma = 0.$$ 

Let $w_{X,Y}^{CLS} \in \mathcal{U}_{Z \cup Y}$, but \notin $H_0^m(\Omega)$, be its CLS approximation, defined as in (3.11). Moreover, let $I_{Z \cup Y}w^*$ denote the unique interpolant of the exact solution $w^* \in H_0^m(\Omega) \subset H^m(\Omega)$ from the trial space $\mathcal{U}_{Z \cup Y} \subset \mathcal{N}_{\Omega, \Phi} = H^m(\Omega)$. Since the stability result in Lemma 16 only applies to functions in the trial space, we shall show that the CLS solution converges to the interpolant in $\mathcal{U}_{Z \cup Y}$.

$$\|w_{X,Y}^{CLS} - w^*\|_{2, \Omega} \leq \|w_{X,Y}^{CLS} - I_{Z \cup Y}w^*\|_{2, \Omega} + \|I_{Z \cup Y}w^* - w^*\|_{2, \Omega} \leq \|w_{X,Y}^{CLS} - I_{Z \cup Y}w^*\|_{2, \Omega} + C_{\Omega, \Phi, L} h_{Z \cup Y}^{m-2}\|w^*\|_{m, \Omega},$$
where the last inequality (by Lemma 13) suggests that we can focus on the
difference $w_{X,Y}^{CLS} - I_{Z \cup Y} w^* \in \mathcal{U}_{Z \cup Y}$, which has zeros at nodes $Y$. Using the
consistency result in Lemma 17, we have

$$
\|w_{X,Y}^{CLS} - I_{Z \cup Y} w^*\|_2, \Omega \leq C_{\Omega, \Phi, \mathcal{L}}(h_X^{d/2} \|\mathcal{L}w_{X,Y}^{CLS} - \mathcal{L}I_{Z \cup Y} w^*\|_X + h_Y^{d/2} \cdot 0) \\
\leq C_{\Omega, \Phi, \mathcal{L}} h_X^{d/2} n_X^{1/2} \rho_X^{d/2} h_Y^{m-2} \|w^*\|_{m, \Omega}.
$$

At this point, we can identify numerical solutions from $\mathcal{U}_{Z \cup Y}$ with discrete
zeros at boundary to approximate the PDE solutions $u^* \in H^m_0(\Omega)$ of homoge-
neous problems that satisfy error estimate:

$$
\|w_{X,Y}^{CLS} - w^*\|_2, \Omega \leq C_{\Omega, \Phi, \mathcal{L}}(h_X^{d/2} n_X^{1/2} \rho_X^{d/2} h_Y^{m-2} \|w^*\|_{m, \Omega}.
$$

### 3.3.2 Nonhomogenous boundary

To show that the same convergence rate also holds for nonhomogenous bound-
dary conditions, it is sufficient to show $u_{X,Y}^{CLS} \to I_{Z \cup Y} u^* \in H^2(\Omega)$ by the same
argument, i.e., $I_{Z \cup Y} u^* \to u^* \in H^2(\Omega)$ at optimal rate. Consider the homoge-
neous problem induced by the PDE in (3.4):

$$
\mathcal{L}w = \mathcal{L}(u - \mathcal{E}g) = f - \mathcal{L}\mathcal{E}g \text{ in } \Omega, \quad w|_{\Gamma} = (u - \mathcal{E}g)|_{\Gamma} = 0.
$$

If $w_{X,Y}^{CLS}$ solves this homogenous problem, then $w_{X,Y}^{CLS} + I_{Z \cup Y} \mathcal{E}g$ is a feasible CLS
candidate for the nonhomogenous one in (3.4). Therefore, by the minimization
property of $u_{X,Y}^{CLS}$, we have

$$
\|\mathcal{L}u_{X,Y}^{CLS} - \mathcal{L}u^*\|_X \leq \|\mathcal{L}(w_{X,Y}^{CLS} + I_{Z \cup Y} \mathcal{E}g) - \mathcal{L}u^*\|_X.
$$

Inserting $\mathcal{L}\mathcal{E}g$ to reconstruct the minimization problem for $w_{X,Y}^{CLS}$, we get

$$
\|\mathcal{L}u_{X,Y}^{CLS} - \mathcal{L}u^*\|_X \leq \|\mathcal{L}w_{X,Y}^{CLS} - \mathcal{L}(u^* - \mathcal{E}g)\|_X + \|\mathcal{L}(I_{Z \cup Y} \mathcal{E}g - \mathcal{E}g)\|_X
\leq \|\mathcal{L}w_{X,Y}^{CLS} - \mathcal{L}(u^* - \mathcal{E}g)\|_X + C_{\Omega, \Phi, \mathcal{L}} n_X^{1/2} \rho_X^{d/2} h_Y^{m-2} \|\mathcal{E}g\|_{m, \Omega}.
$$

Now, the consistency result for homogenous problem (Lemma 17) can be ap-
piled, i.e,

$$
\|\mathcal{L}w_{X,Y}^{CLS} - \mathcal{L}(u^* - \mathcal{E}g)\|_X \leq C_{\Omega, \Phi, \mathcal{L}} n_X^{1/2} \rho_X^{d/2} h_Y^{m-2} \|u^* - \mathcal{E}g\|_{m, \Omega}.
$$
By Lemma 13, we have

\[
\| \mathcal{L}u_{X,Y}^{CLS} - \mathcal{L}I_{Z\cup Y}u^* \|_X \\
\leq \| \mathcal{L}u_{X,Y}^{CLS} - \mathcal{L}u^* \|_X + \| \mathcal{L}u^* - \mathcal{L}I_{Z\cup Y}u^* \|_X \\
\leq C_{\Omega,\phi,\mathcal{L}}n_{X}^{1/2}\rho_{X}^{d/2}h_{Z\cup Y}^{m-2}(\|u^* - \mathcal{E}g\|_{m,\Omega} + \|\mathcal{E}g\|_{m,\Omega} + \|u^*\|_{m,\Omega}) \\
\leq C_{\Omega,\phi,\mathcal{L}}n_{X}^{1/2}\rho_{X}^{d/2}h_{Z\cup Y}^{m-2}(\|\mathcal{E}g\|_{m,\Omega} + \|u^*\|_{m,\Omega}).
\]

Suppose \( \Omega \) satisfies Assumption 5; the trace \( \mathcal{T} \) and extension \( \mathcal{E} \) operators are continuous and hence bounded. So, we have

\[
\|\mathcal{E}g\|_{m,\Omega} = \|\mathcal{E} \circ \mathcal{T}u^*\|_{m,\Omega} \leq C_{\Omega}\|u^*\|_{m,\Omega}.
\]

By calling the stability result in Lemma 16 (that applies to functions in the trial space only), it is straightforward to complete proof of Theorem 10:

\[
\|u_{X,Y}^{CLS} - u^*\|_{2,\Omega} \leq \|I_{Z\cup Y}u^* - u^*\|_{2,\Omega} + \|u_{X,Y}^{CLS} - I_{Z\cup Y}u^*\|_{2,\Omega} \\
\leq \|I_{Z\cup Y}u^* - u^*\|_{2,\Omega} + C_{\Omega,\mathcal{L}}h_{X}^{d/2}\|\mathcal{L}u_{X,Y}^{CLS} - \mathcal{L}I_{Z\cup Y}u^*\|_X \\
\leq C_{\Omega,\phi,\mathcal{L}}(1 + h_{X}^{d/2}n_{X}^{1/2}\rho_{X}^{d/2})h_{Z\cup Y}^{m-2}\|u^*\|_{m,\Omega}.
\]

Under the assumption that \( X \) is asymptotically quasi-uniform, and since \( n_{X} \sim q_{X}^{-d} \), \( C_{\Omega,\phi,\mathcal{L}}(1 + h_{X}^{d/2}n_{X}^{1/2}\rho_{X}^{d/2}) \) can be simplified to \( C_{\Omega,\phi,\mathcal{L}}\gamma_{X} \) that also depends on \( \gamma_{X} \).

### 3.4 Convergence for WLS

Instead of a specific weight, we will consider a class of weighted least-squares formulations by a simple inequality.

**Lemma 18.** Let \( a, b > 0 \), \( 0 < \epsilon < 1 \), and \( 0 \leq \theta \leq 2 \). Then the following inequalities hold:

\[
(\epsilon a + b)^2 \leq 2(\epsilon^\theta a^2 + b^2).
\]

**Proof.** Consider \( 0 \leq \theta/2 \leq 1 \). From \((\epsilon a + b)^2 \leq 2(\epsilon^2 a^2 + b^2)\) and \( \epsilon \leq \epsilon^{\theta/2} \), we have \((\epsilon a + b)^2 \leq 2(\epsilon^\theta a^2 + b^2)\). \(\square\)
Lemma 19 (H²-Stability). Suppose the assumptions in Lemma 16 hold. If \( h_X \leq h_Y < 1 \), then there exists a constant \( C_{\Omega, \Phi, \mathcal{L}} \), depending only on \( \Omega \), \( \Phi \), and \( \mathcal{L} \) such that
\[
\|u\|_{2, \Omega} \leq C_{\Omega, \Phi, \mathcal{L}} \left( \frac{h_X}{h_Y} \right)^{d/4} h_Y^{d/2 - (2 - \theta)} \left( \|\mathcal{L}u\|_X^2 + \left( \frac{h_Y}{h_X} \right)^{d/2} h_Y^{-2\theta} \|u\|_Y^2 \right)^{1/2}
\]
holds for all \( 0 \leq \theta \leq 2 \) and all \( u \in \mathcal{U}_{Z \cup Y} \) for any finite sets \( X \subset \Omega \) and \( Y \subset \Gamma \) with sufficiently small relative fill distances \( h_X/h_Z \) and \( h_Y/h_Z \).

Proof. The CLS stability in Lemma 16 has to be further modified to suit the need of WLS. With the denseness requirement (3.18), let us start with
\[
\|u\|_{2, \Omega} \leq C_{\Omega, \Phi, \mathcal{L}} \left( h_X^{d/2} \|\mathcal{L}u\|_X + h_Y^{d/2} \|u\|_Y \right).
\]
(3.19)
We want to obtain a stability estimate with discrete sum of squares. Rewrite (3.19) as
\[
\|u\|_{2, \Omega}^2 \leq C_{\Omega, \Phi, \mathcal{L}} h_Y^{d/4} \left( \epsilon \|\mathcal{L}u\|_X + \|u\|_Y \right)^2 \quad \text{with} \quad \epsilon = \left( \frac{h_X}{h_Y} \right)^{d/2} h_Y^2.
\]
Note that having \( \epsilon < 1 \) is a very mild requirement, for example \( h_X \leq h_Y < 1 \), and will not be an obstacle between theories and practice. By Lemma 18, we have
\[
\|u\|_{2, \Omega} \leq \left( C_{\Omega, \Phi, \mathcal{L}} h_Y^{d/4} \left( \epsilon \|\mathcal{L}u\|_X + \|u\|_Y \right) \right)^{1/2} \leq C_{\Omega, \Phi, \mathcal{L}} h_Y^{d/2 - 2} \epsilon^{\theta/2} \left( \|\mathcal{L}u\|_X^2 + \epsilon^{-\theta} \|u\|_Y^2 \right)^{1/2},
\]
for any \( 0 \leq \theta \leq 2 \). Substituting \( \epsilon \) back yields
\[
\|u\|_{2, \Omega} \leq C_{\Omega, \Phi, \mathcal{L}} h_Y^{d/2 - 2} \left( \left( h_X/h_Y \right)^{d/2} h_Y^{2\theta} \left( \|\mathcal{L}u\|_X^2 + \left( h_X/h_Y \right)^{d/2} h_Y^{2\theta} \right) \right)^{1/2},
\]
and we obtain the desired WLS stability after simplification.

Lemma 20 (Consistency). For any \( W > 0 \), define a functional \( J_W : H^m(\Omega) \to \mathbb{R} \) by \( J_W(u) := \left( \|\mathcal{L}u\|_X^2 + W \|u\|_Y^2 \right)^{1/2} \). Suppose the assumptions in Lemma 17 hold. Then, we have
\[
\min_{v \in \mathcal{U}_{Z \cup Y}} J_W(v - u^*) \leq C_{\Omega, \Phi, \mathcal{L}} h_X^{1/2} \rho_X^{d/2} h_Y^{m-2} \|u^*\|_{m, \Omega},
\]
for any \( u^* \in H^m(\Omega) \).
Proof. Again, we compare the minimizer \( v^* \) with the interpolant \( I_{Z^U}u^* \) in \( U_{Z^U} \):

\[
J_W^2(v^* - u^*) \leq J_W^2(I_{Z^U}u^* - u^*)
= \| \mathcal{L}I_{Z^U}u^* - \mathcal{L}u^* \|^2_X + \| I_{Z^U}u^* - u^* \|^2_Y,
\]

where the last term vanishes due to the zeros of \( I_{Z^U}u^* - u^* \) at \( Y \). Therefore, we have an upper bound for the minimum of \( J_W \) by (3.7),

\[
J_W(v^* - u^*) \leq \| I_{Z^U}u^* - u^* \|_{2,X}.
\]

The lemma follows after an application of interpolation estimate (Lemma 14).

With both consistency and stability results, we can now prove the convergence of a class of WLS solutions defined by (3.12). By similar arguments used in Section 3.3, we only need to show that the WLS solution converges to the interpolant \( I_{Z^U}u^* \) of the exact solution \( u^* \) from the trial space \( U_{Z^U} \). For \( 0 \leq \theta \leq 2 \), consider the functional

\[
J_{W(\theta)}(u) := (\| \mathcal{L}u \|^2_X + W(\theta)\| u \|^2_Y)^{1/2} \quad \text{with} \quad W(\theta) := (h_Y/h_X)^{d\theta/2}h_Y^{-2\theta}. \quad (3.20)
\]

Applying the results of Lemmas 19 and 20, we have the WLS solution convergence within the trial space:

\[
\| u_{X,Y,Z^U}^{WLS,\theta} - I_{Z^U}u^* \|_{2,\Omega} \leq C_{\Omega,\phi,\mathcal{L}}(h_X/h_Y)^{d\theta/4}h_Y^{d/2(2-\theta)}J_{W(\theta)}(u_{X,Y,Z^U}^{WLS,\theta} - I_{Z^U}u^*) \leq C_{\Omega,\phi,\mathcal{L}}(h_X/h_Y)^{d\theta/4}h_Y^{d/2(2-\theta)}n_X^{1/2}n_X^{d/2}h_{Z^U}^{m-2}\| u^* \|_{m,\Omega}.
\]

Now we can compare the difference between WLS solution and the exact solution,

\[
\| u_{X,Y,Z^U}^{WLS,\theta} - u^* \|_{2,\Omega} \leq \| u_{X,Y,Z^U}^{WLS,\theta} - u^* \|_{2,\Omega} + \| u_{X,Y,Z^U}^{WLS,\theta} - I_{Z^U}u^* \|_{2,\Omega} \leq C_{\Omega,\phi,\mathcal{L}}(1 + h_Y^{-(2-\theta)(d-4)/4}h_X^{d\theta/4}n_X^{1/2}n_X^{d/2}h_{Z^U}^{m-2}\| u^* \|_{m,\Omega}) \leq C_{\Omega,\phi,\mathcal{L}}(1 + C_{\gamma X}h_X^{-(2-\theta)(d-4)/4}h_Y^{(2-\theta)(d-4)/4}h_{Z^U}^{m-2}\| u^* \|_{m,\Omega}) \leq C_{\Omega,\phi,\mathcal{L},\gamma X}(1 + h_X^{-(2-\theta)/4}h_Y^{(2-\theta)(d-4)/4}h_{Z^U}^{m-2}\| u^* \|_{m,\Omega}),
\]

55
for $0 \leq \theta \leq 2$. The last holds because $h^{d/2}n_X^{1/2}\rho_X^{d/2}$ can be bounded by some $C_{\gamma_X}$. Moreover, the constant 1, coming from $\|I_{Z\cup Y}u^* - u^*\|_{2,\Omega}$, is absolutely necessary or else the error bound will allow arbitrarily fast convergence with respect to $h_X \to 0$ for some $\theta$ and $d$.

It is obvious that $\theta = 2$ maximizes the convergence rate:

$$\|u_{X,Y,2}^{WLS} - I_{Z\cup Y}u^*\|_{2,\Omega} \leq C_{\Omega,\Phi,\mathcal{L},\gamma_X}h_X^{m-2}\|u^*\|_{m,\Omega}.$$  

The CLS and the optimal WLS($\theta = 2$) formulation share convergence estimates of the same form. They both match the convergence estimate of the interpolant exactly, that in turn confirms their optimality. To complete proving Theorem 11, we consider the stability for $\theta = 2$ and Lemma 19 gives

$$\|u\|_{2,\Omega} \leq C\Omega,\Phi,\mathcal{L}h_X^{d/2}(\|Lu\|_{2,X}^2 + (h_Y/h_X)^d h_Y^{-2}\|u\|_{Y}^2)^{1/2}$$

$$\leq C\Omega,\Phi,\mathcal{L}h_X^{d/2}(\|Lu\|_{2,X}^2 + (h_Y/h_X)^d h_Y^{-2\theta}\|u\|_{Y}^2)^{1/2},$$

for any $\theta \geq 2$ as long as $h_Y < 1$. Extend the definition of functional $J_{W(\theta)}$ to $\theta \geq 2$ by the same definition as in (3.20). Then, for any $u \in H^m(\Omega)$, we have

$$J_{\theta_1}(u) \leq J_{\theta_2}(u), \quad \text{for } 2 \leq \theta_1 \leq \theta_2 \leq \infty.$$  

Since the CLS formulation is equivalent to the WLS with $\theta = \infty$, for any $\theta \geq 2$, we have

$$\min_{v \in I_{Z\cup Y}} J_{W(\theta)}(v - u^*) \leq J_{W(\theta)}(u_{X,Y}^{CLS} - u^*) \leq J_{W(\infty)}(u_{X,Y}^{CLS} - u^*),$$

where the last term is minimal by the definition of CLS solution. Theorem 11 can now be concluded based on Theorem 10.

### 3.5 Optimal WLS weighting revisited

Hu, Chen and et al. (Hu et al., 2007) showed by scaling analysis that the optimal weighting for WLS is $n_Z^2$ for bounded $\Omega \subset \mathbb{R}^2$. This corresponds to $\theta = 1$ (instead of the optimal $\theta = 2$ found in the previous section) in our
notation with all fill distances \( h_X, h_Y, \) and \( h_Z \) are of the same magnitude. To ensure our proven theories are consistent with the previous findings, there are two things we need to care of. Firstly, if we assume \( h_X \sim h_Y \) on top of all other denseness requirements, then the error bound in Theorem 11 reduces to

\[
\|u_{X,Y,Z,Y}^{WLS,\theta} - u^*\|_{2,\Omega} \leq C_{\Omega,\Phi,\xi,\gamma} h_Z^{m-2}\|u^*\|_{m,\Omega}, \quad \text{for } d = 2, 0 \leq \theta \leq \infty.
\]

In other words, for bounded \( \Omega \subset \mathbb{R}^2 \), any weighted least squares can converge at optimal rate. Secondly, the trial space used in (Hu et al., 2007) is a smaller \( \mathcal{U}_Z \) rather than the one including boundary collocation points \( \mathcal{U}_{Z,Y} \) we used in Theorem 11. In the rest of this section, we will focus on the WLS convergence in this smaller trial space and prove Theorem 12.

To begin, let us return to the proof for WLS consistency (Lemma 20) but restrict the approximation in the smaller trial space \( \mathcal{U}_Z \), within which the stability result in Lemma 19 remains valid. However, we can only compare the minimizer \( v^* \in \mathcal{U}_Z \) with the interpolant \( I_Z u^* \in \mathcal{U}_Z \) to the exact solution \( u^* \in H^m(\Omega) \):

\[
\min_{v \in \mathcal{U}_Z} J^2_W(v - u^*) \leq J^2_W(I_Z u^* - u^*) = \|\mathcal{L}I_Z u^* - \mathcal{L}u^*\|_X^2 + W\|I_Z u^* - u^*\|_Y^2.
\]

To handle the boundary term, which has no particular pattern of zeros, we want to bound the \( \ell_2(Y) \) norm on the boundary by some \( \ell_2(\tilde{Z} \cup Y) \) norm in the interior (like the trace theorem does). For any subset \( \tilde{Z} \subseteq Z \), applying the interpolation estimate (Lemma 14) gives:

\[
\|I_Z u^* - u^*\|_Y = \|I_Z u^* - u^*\|_{\tilde{Z} \cup Y} \leq C_{\Omega,\Phi,\gamma_Y^{1/2} h_{\tilde{Z} \cup Y}^{d/2} h_Z^m}\|u^*\|_{m,\Omega}.
\]

We already assumed \( Z \) is quasi-uniform in Assumption 9. Let us further assume that \( Y \) is also quasi-uniform on \( \Gamma \) and it satisfies (3.10) with some constant \( \gamma_Y > 1 \) and \( h_Y \leq h_Z \). Consider the subset \( \tilde{Z} \subseteq Z \) defined as \( \tilde{Z} := \{z \in Z \cap \Omega_{h_Z}\} \) where \( \Omega_\varepsilon := \{z \in \Omega : \text{dist}(z - \Gamma) > \varepsilon\} \) for any \( \varepsilon > 0 \). For sufficiently dense \( Y \), we have control on the denseness of the set \( \tilde{Z} \cup Y \). By
(Fuselier and Wright, 2012, Thm.6), the denseness measures of $Y$ on $\Gamma$ and in $\Omega$ (or $\mathbb{R}^d$ in the original theorem) will eventually be proportional, i.e., $h_{Y, \Gamma} \sim h_{Y, \Omega}$ and $q_{Y, \Gamma} \sim q_{Y, \Omega}$. If $\Omega$ is a thin domain, the denseness requirement on $Y$ will be higher.

With $h_Y$ small enough, we have

$$
\min(q_Z, q_Y) \leq q_{\tilde{Z} \cup Y} \leq \left( \sup_{\zeta \in \Omega_{h_Z}} + \sup_{\zeta \in \Omega \setminus \Omega_{h_Z}} \right) \min_{z \in \tilde{Z} \cup Y} \|z - \zeta\|_{L^2(\mathbb{R}^d)} \leq h_Z + (h_Z + h_{Y, \Omega}).
$$

It is now clear that the set $\tilde{Z} \cup Y$ is also quasi-uniform with respect to some parameter $\gamma_{\tilde{Z} \cup Y}$ that depends on $\gamma_Z$ and $\gamma_Y$. Hence, we can bound $\rho_{\tilde{Z} \cup Y}$ by some generic constant $C_{\gamma_Y, \gamma_Z}$. To simplify the term $n_{\tilde{Z} \cup Y}$, consider

$$
n_{\tilde{Z} \cup Y} \leq n_Z + n_Y \leq C_{\gamma_Y, \gamma_Z} (h_Z^{-d} + h_Y^{-(d-1)}) \leq C'_{\gamma_Y, \gamma_Z} (h_Y^{-d} + h_Y^{d+1}),
$$

and, since we assumed $h_Y < 1$, we have $n_{\tilde{Z} \cup Y} \leq C_{\gamma_Y, \gamma_Z} h_Y^{-d}$.

Together, we have

$$
\|I_Z u^* - u^*\|_Y \leq C_{\Omega, \Phi, \gamma_Y, \gamma_Z} h_Y^{-d/2} h_Z^m \|u^*\|_{m, \Omega}.
$$

The PDE residual at $X$ can be dealt with similarly:

$$
\|\mathcal{L} u^* - \mathcal{L}I_Z u^*\|_X \leq C_{\Omega, \Phi, \ell, \gamma_X} h_X^{-d/2} h_Z^m \|u^*\|_{m, \Omega} \leq C_{\Omega, \Phi, \ell, \gamma_X} h_X^{-d/2} h_Z^m \|u^*\|_{m, \Omega},
$$

and we have

$$
\min_{v \in \mathcal{U}_Z} J^2_W (u^* - v) \leq C_{\Omega, \Phi, \ell, \gamma_X} (h_X^{-d/2} h_Z^m \|u^*\|_{m, \Omega})^2 + W \left( C_{\Omega, \Phi, \gamma_Y, \gamma_Z} h_Y^{-d/2} h_Z^m \|u^*\|_{m, \Omega} \right)^2.
$$
or, square-rooting both sides to yield

$$\min_{v \in U} J_W(u^* - v) \leq C_{\Omega, \Phi, \mathcal{L}, \vec{\gamma}} \left( (h_X^{-d/2})^2 + W(h_Y^{-d/2} h_Z^2)^2 \right)^{1/2} h_Z^{m-2} \|u^*\|_{m, \Omega},$$

with \( \vec{\gamma} = [\gamma_X, \gamma_Y, \gamma_Z] \) in the constant. By the inequality \( \sqrt{a^2 + b^2} \leq a + b \) for \( a, b \geq 0 \), we conclude that

$$\min_{v \in U} J_W(u^* - v) \leq C_{\Omega, \Phi, \mathcal{L}, \vec{\gamma}} \left( h_X^{-d/2} + W^{1/2} h_Y^{-d/2} h_Z^2 \right) h_Z^{m-2} \|u^*\|_{m, \Omega}. $$

Now, putting stability and \( W = (h_Y/h_X)^{d/2} h_Y^{-2g} \) into account, we get the error bound

$$\|u_{X,Y,Z}^{WLS,\theta} - u^*\|_{2, \Omega} \leq \|I_Z u^* - u^*\|_{2, \Omega} + \|u_{X,Y,Z}^{WLS,\theta} - I_Z u^*\|_{2, \Omega} \leq C_{\Omega, \Phi, h_Z^{m-2}} \|u^*\|_{m, \Omega} + C_{\Omega, \Phi} h_Z^{-2} \|u^*\|_{m, \Omega} \leq C_{\Omega, \Phi} \left( 1 + h_X^{(g-2)/4} h_Y^{(g-2)(d-4)/4} + h_Y^2 h_Z^2 \right) h_Z^{m-2} \|u^*\|_{m, \Omega}. $$

Therefore, Theorem 12 is proven. Without \( Y \) in the trial centers to annihilate the boundary collocation, we got one extra higher-order term \( h_Y^2 h_Z^2 \). The weight suggested in (Hu et al., 2007) is optimal for \( \Omega \subset \mathbb{R}^2 \), as well as all the others.

### 3.6 Numerical demonstrations

We test the proposed formulations in \( \Omega = [-1, 1]^2 \). Discretization is done by using regular centers \( Z \) with \( n_Z = 11^2, 16^2, \ldots, 36^2 \). Collocation points \( X \) (strictly in the interior) and \( Y \) are constructed similarly with \( h_X = \delta_i h_Z \) and \( h_Y = \delta_b h_Z \) with \( \delta_i = 1, 1/2, 1/3 \) and \( \delta_b = 1, 1/2 \) such that \( Z \subseteq X \) and \((Z \cap \Gamma) \subseteq Y \) respectively. The reported errors are calculated using a fine 100^2 grid.

In matrix form, collocation conditions for the PDE and boundary condition can be written as

$$K_{\mathcal{L}, X} \lambda = f_{|X} \quad \text{and} \quad K_{\mathcal{E}, Y} \lambda = g_{|Y},$$
respectively, with entries \([K_{L,X}]_{ij} = \mathcal{L}\Phi(x_i - z_j)\) and \([K_{B,Y}]_{ij} = \Phi(y_i - z_j)\) for \(x_i \in X\) and \(y_i \in Y\). Both resultant matrices have \(n_Z + n_Y\) (and \(n_Z\)) columns for trial space \(U_{Z \cup Y}\) (and \(U_Z\)) corresponding to each \(z_j\) from the trial space. In the CLS approach (3.11), the constraints at \(Y\) are enforced using the null space matrix of the boundary collocation matrix, denoted by \(N_{B,Y} := \text{null}(K_{B,Y})\), as in (Ling and Hon, 2005), so that the unknown coefficient is expressed in the form

\[
\lambda = N_{B,Y} \gamma + K_{B,Y}^\dagger g_{|Y},
\]

for some new unknown \(\gamma\), which can be found by solving

\[
K_{L,X} N_{B,Y} \gamma = f_{|X} - K_{L,X} K_{B,Y}^\dagger g_{|Y}.
\]

In all WLS(\(\theta\)) formulations, with LS weighting specified by \(W(\theta)\) in (3.12), the unknown coefficient \(\lambda\) is obtained by solving the following overdetermined system

\[
\begin{bmatrix}
K_{L,X} \\
W(\theta) K_{B,Y}
\end{bmatrix}
\lambda
=
\begin{bmatrix}
f_{|X} \\
W(\theta) g_{|Y}
\end{bmatrix}
\]

with Matlab’s \texttt{mldivide} in the least-squares sense. For all computations in this section, we did not employ any technique to deal with the problem of ill-conditioning unless specified otherwise, i.e., when we employ the stable RBF-QR decomposition for the Gaussian basis. To deal with the numerical instability, readers are referred to our trial subspace selection techniques (Ling and Schaback, 2009).

### 3.6.1 How dense is dense

We consider a Poisson problem with smooth solution \(u^*(x, y) = \sin(\frac{\pi x}{2}) \cos(\frac{\pi y}{2})\) and the Dirichlet boundary value is generated from \(u^*\). We cast the CLS formulation with the unscaled Whittle-Matérn-Sobolev kernels that reproduce \(H^m(\Omega)\) with \(m = 3, \ldots, 6\). Note that convergence theories require \(m \geq 5\) for \(\Omega \subset \mathbb{R}^2\).
Figure 3.3 compactly shows all convergence profiles in $H^2(\Omega)$ and $L^2(\Omega)$ at a glance. To begin, let us focus on the $H^2(\Omega)$ errors on the left side of Figure 3.3. Generally speaking, for all tested smoothness $m$, all collocation settings demonstrate an $m - 2$ convergence and match with the estimates in Theorem 10; this also includes the original Kansa formulation with $Z = X \cup Y$. It is obvious that the error profiles for each tested $m$ is split into two groups. The least accurate groups (i.e., the group above) correspond to $h_X = h_Z$. Without over-testing the PDE, this setting would probably fail the denseness requirement (3.18) but yet allow convergence at the optimal rate. All errors reduce at a rather constant rate, except that we can see two unstable profiles in the cases of $m = 6$. These numerical instabilities correspond to the two cases with large numbers of boundary collocations; $(h_X, h_Y) = (h_Z/2, h_Z/2)$ and $(h_X, h_Y) = (h_Z/3, h_Z/2)$.

As one would expect, the $L^2(\Omega)$ error profiles, on the right side of Figure 3.3, show exactly two extra orders and achieve an $m$-order convergence before numerical instability kicks in. We can clearly see that higher smoothness typically suffers the effects of ill-conditioning more. Error reduction reaches a valley, a.k.a. numerical optimal, and then bounds up. In the case of $m = 6$, any over-testing causes the accuracy to drop and only the original Kansa square setting shows a straight error profile in our test range of $h_Z$.

### 3.6.2 CLS convergence in trial space $U_Z$

Putting the theoretical optimal aside, we are interested in the CLS convergence for the two trial spaces $U_Z$ and $U_{Z \cup Y}$. The former is smaller and more practical. Now, we turn our focus to the CLS formulation in the smaller trial space $U_Z$. Linear algebra says that if $n_Z < n_Y$, then we may not be able to find nontrivial functions from $U_Z$ with zeros at $Y$. However, one can observe numerically that the CLS hardly runs into trouble when it is cast in this smaller trial space. Numerically, as $h_Y \to 0$, the rank of the boundary collocation matrix is bounded; for example, for $n_Z = 21^2$ with finer and finer $Y$, we can see that the
rank of the boundary matrix is numerically bounded:

<table>
<thead>
<tr>
<th>$U_{Z,Y}$</th>
<th>$U_Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_Y$</td>
<td>rank($K_{B,Y}$)</td>
</tr>
<tr>
<td>80</td>
<td>80</td>
</tr>
<tr>
<td>160</td>
<td>104</td>
</tr>
<tr>
<td>244</td>
<td>108</td>
</tr>
<tr>
<td>328</td>
<td>100</td>
</tr>
</tbody>
</table>

Figure 3.4 shows the error profiles for the CLS performance in $U_Z$ with all other settings identical to those in Figure 3.3. Comparing the CLS in the two trial spaces, we observe that optimal convergence is also possible in $U_Z$ but only for small enough $h_Z$. The CLS accuracy can “catch up” when the numerical rank of $K_{B,Y}$ is relatively insignificant compared to $n_Z$. Therefore, the larger the rank($K_{B,Y}$) the longer CLS takes to achieve optimal convergence. By using a smaller trial space, we not only gain computational efficiency but suffer less ill-conditioning. There is no obvious accuracy rebound in $H^2(\Omega)$ and that in $L^2(\Omega)$ appears later with smaller magnitude. In our next demonstration, we will see that $U_Z$ only makes CLS convergence lag behind, but not to any other WLS formulations.

### 3.6.3 Numerically optimal weight for WLS

Now we consider the WLS($\theta$) formulation with $\theta \in \{\infty, 0, 0.5, 1, 2\}$, in which WLS($\theta = \infty$) is equivalent to the CLS. We set $h_X = h_Y = h_Z/2$ and hence the LS weighting tested are $W(\theta) = 1$, $n_Z$, $n_Z^2$ and $n_Z^4$. Theorem 11 and Theorem 12 ensure all other tested WLS are optimally convergent in both trial spaces. Figure 3.5 shows the error profiles associated with Whittle-Matérn-Sobolev kernels of various smoothness. The estimated convergence rates shown in the legends are obtained from least-squares fitting to all data; if the convergence profile is not “straight” enough, the corresponding estimate is not trustworthy.
Figure 3.1: Schematic point sets, collocations $X$ and $Y$ (left), and trial $Z$ (right), used to solve various PDEs.

From Figure 3.5, we immediately see that there is no benefit at all (in terms of both efficiency and accuracy) to go for the unweighted LS formulation. Unlike the CLS in $U_Z$, WLS with finite weight does not suffer the lag in convergence. However, if we focus on the case ($m = 4, \theta = 2$) in $U_Z$, we can see that over-weighted boundary collocations will still hurt the accuracy, but not the convergence behavior. By comparing the left and right plots in each row of Figure 3.5, we see that there are some weightings for each smoothness $m$ that allow similar accuracy and convergence rate in both trial spaces. But again, using $U_Z$ is computationally cheaper.

To further verify these observations, we change the $n_X$ regular collocation points to scattered sets using the Halton sequence; see Figure 3.1 for one of these point sets. Boundary collocation points remain regular with $h_Y = h_Z/2$ and we employ the Whittle-Matérn-Sobolev kernel with $m = 4$. Figure 3.6 reports the error profiles from three different PDEs, all with the Matlab’s `peaks(3x,3y)` as exact solution. These results should be compared to the first row ($m = 4$) of Figure 3.5 and the convergence patterns are very similar. Yet, there are some minor, but notable differences.

Based on these test results, the moderate $\theta = 0.5$ is the best weighting in practice; it is numerically more stable and is as accurate as CLS in the large trial space.
3.6.4 Some observations for GA and MQ

Let us begin with two CLS approximations obtained by using the unscaled Gaussian kernel, see Figure 3.2. We generate the trial space $U_Z$ using $n_Z = 36^2$ centers. Collocations are enforced on regular $X$ and $Y$ with $h_X = h_Y = h_Z/2$. We then solve two Poisson problems with different exact solutions $u^* = \text{peaks}(x, y)$ (zoom-in peak) and $u^* = \text{peaks}(3x, 3y)$ (full peak). Both systems share the same Kansa matrix and only differ by the right-hand vectors $f|X$ and $g|Y$. Although both systems have exactly the same condition number, the resulting accuracy has a huge difference: 8.1E-12 and 3.5E-3 $L^2(\Omega)$ error respectively, for the zoom-in and full peaks. One could argue that the Gaussian native space is relatively small and it may not contain the full peak function that causes low accuracy. To know for sure, a change of stable basis (a.k.a. RBF-QR algorithm (Fasshauer and McCourt, 2012; Fornberg et al., 2011)) can give us a clearer picture. Using some downloadable Matlab codes (Larsson, ), we can cast the CLS formulation completely in the new stable basis and yield new $L^2(\Omega)$ errors, 5.7E-8 and 6.3E-9 respectively for the two exact solutions. For the zoom-in peak, accuracy drops, which can be explained by the truncation error within the RBF-QR algorithm. Whereas, the huge accuracy improvement suggests there is a good candidate in the native space of Gaussian to approxi-
mate the full peak function. In Figure 3.7, we show the error profiles for direct Gaussian (GA) and stable basis (RBF-QR) for both solutions. When solving the zoom-in peak, GA can provide highly accurate approximation and its error stagnates for large \( n_Z \); adding RBF-QR (as is without modification) to the algorithm will introduce numerical instability. The situation is very different in the full peak when GA fails to converge; having RBF-QR brings convergence back in the game. We remark that the RBF-QR algorithm prefers flatter (than our unscaled) Gaussian basis for both accuracy and efficiency. Moreover, some of the highly accurate approximations in RBF-QR suggest that it is highly possible to properly truncate the Gaussian expansion in order to couple with the CLS and WLS approaches. This is out of the scope of this work, but worth some further investigation.

Our demonstration will end with the results of the unscaled multiquadrics (MQ) kernel in Figure 3.8. While the full peak function is giving the Gaussian kernel trouble, the multiquadrics is doing very well. The CLS and WLS with \( \theta = 0.5 \) and 1 all converge at an estimated rate of 20. Also, the CLS convergence lag in \( U_Z \) is not at all noticeable. Turning to the less varying zoom-in peak, the same MQ-PDE resultant matrix only yields an 8th-order convergence. This example again confirms that condition number alone cannot be used to predetermine the accuracy or convergence rate of Kansa related methods using GA or MQ basis.

**Conclusion**

We prove some error estimates for a constraint least-squares and a class of weighted least-squares strong-form RBF collocation formulations for solving general second order elliptic problem with nonhomogenous Dirichlet boundary condition. All analysis is carried out in Hilbert spaces so that both PDE and RBF theories apply. We show that the CLS and WLS formulations using kernels that reproduce \( H^m(\Omega) \) can converge at the optimal \( h^{m-2} \) in \( H^2(\Omega) \).
Besides some standard smoothness assumptions for high order convergence, the sets of collocation points have to be relatively dense in comparison to the set of trial centers for the convergence theories to hold. All our formulations become the original Kansa method if one imposes conditions on centers (i.e., $X \cup Y = Z$). Although general convergence theories for the original Kansa approach is impossible, our theories apply if the given PDE has a small generic constant in the denseness requirement (3.18) to allow $h_X = h_Y = h_Z$. This could be a reason why researchers keep observing the optimal convergence rate from the Kansa method.

We verify by numerical examples that there are many convergent formulations for $\Omega \subset \mathbb{R}^2$ enjoy the optimal convergence rate. We thoroughly study the performance of Whittle-Matérn-Sobolev kernels in two trial spaces numerically. The larger space that includes all boundary collocation points as trial centers is more theoretically sound (in the sense of the range of optimal weighting), whereas the small one is computationally more efficient. Taking both accuracy and efficiency into consideration, casting WLS in the small trial space with a moderate weight (i.e. $\theta = 0.5$ or $1$) consistently yields competitive accuracy and numerical stability. This recommendation for WLS also extends to the commonly used Gaussian and multiquadrics kernels, which do not reproduce Sobolev space as the theories require. We also provide a brief demonstration for using the RBF-QR algorithm on our formulations to hint at possibilities for future researches.
Figure 3.3: $H^2(\Omega)$ (left) and $L^2(\Omega)$ (right) error profiles for CLS in $U_{Z,Y}$ using Whittle-Matérn-Sobolev kernels of order $m = 3, \ldots, 6$ (green, blue, black, and red).

Figure 3.4: Error profiles for CLS in $U_Z$ corresponding to Figure 3.3.
Figure 3.5: $H^2(\Omega)$ error profiles of WLS($\theta$) in $\mathcal{U}_{Z\cup Y}$ (left) and in $\mathcal{U}_Z$ (right) using Whittle-Matérn-Sobolev kernels of order $m = 4, 5, 6$. 
Figure 3.6: $H^2(\Omega)$ error profiles of WLS($\theta$) in $U_{Z\cup Y}$ (left) and in $U_Z$ (right) using Whittle-Matérn-Sobolev kernels of order $m = 4$ for three PDEs.
Figure 3.7: $L^2(\Omega)$ error of CLS in $\mathcal{U}_Z$ using the unscaled Gaussian kernel for a Poisson problem with two different solutions $u^\ast$. 
Figure 3.8: $L^2(\Omega)$ error for CLS using the unscaled multiquadrics kernel corresponding to Figure 3.7.
Chapter 4

Convergent meshless collocation formulation for partial differential equations on surfaces

We considered second order elliptic partial differential equation on smooth surface. We proved the embedding conditions for solving Laplace-Beltrami operator are derivative free. i.e., It does not require to differentiate the normal vector. We solve the proposed strong-form collocation embedding method in the least square sense. We proved an $L^2$ error estimate for this least-square solution with some denseness requirement. Numerical demonstration have been given to show that the denseness requirement can be improved. We verified by numerics that the $L_2$ error estimate by using Whittle-Matérn-Sobolev kernels. Time-dependent partial differential equation on surface was also considered. We exhibit the pattern formation by solving reaction-diffusion equation.

4.1 Introduction

Solving partial differential equations (PDEs) on surfaces have wide applications in imaging processing, computer graphics (Turk, 1991; Bertalmio et al., 2000), mathematical physics, fluid dynamics and mathematical biology (Chaplain
et al., 2001; Varea et al., 1999). In the literature, various kinds of methods for solving PDEs on surfaces can be found. Typically, these methods can be classified into non-embedding and embedding types. For non-embedding methods, some sort of parametrization of the surface and discretization of the surface differential operator are necessary. This may lead to distortions as well as singularities in the surface (Floater and Hormann, 2005; Lui et al., 2005; Stam, 2003; Witkin and Kass, 1991). Moreover, non-embedding methods are generally of low order accuracy.

For embedding methods, an embedded problem is posed in spaces at least one dimension higher than that of the original problem. The PDEs will be solved in the embedding space as a subset of Euclidean space. Then, the solution of the original problem will be obtained by restriction of the solution of embedding problem on the surface. As the embedded problem are posed on the $\mathbb{R}^d$, standard numerical solvers such as finite difference method, finite volume method and finite element method can be applied directly.

In 2008, Ruuth et al. (Ruuth and Merriman, 2008) proposed an embedding method, a.k.a. the closest point method, for PDEs on surfaces. The embedding is built on a closest point mapping $cp$ which map each point $x \in \mathbb{R}^d$ in the embedded space onto the surface $cp(x) \in S$ so that $cp(x)$ is closest to $x$. The closest point mapping $cp$ play an important role in the embedding and yields an orthogonal extension along the norm direction of the surface. Once the embedding has been established, the surface gradient operator and the Laplacian-Beltrami operator can be simply replaced by the usual gradient operator and usual Laplacian operator in Euclidean space. The embedded PDE can be solved by any numerical solvers developed in Euclidean space. As examples, second order accurate numerical solution is obtained by standard finite difference method along with carefully implemented interpolation between points on surface and computational grids, (Ruuth and Merriman, 2008). Based on the idea of closest point method, Piret (Piret, 2012) developed an orthogonal gradient method to avoid the interpolation. The orthogonal gradient method
distribute data points orthogonal to the surface, hence, have identical function values under the closest point mapping. The trade-off is that one must now work with irregular data points and this is where meshless methods come into the play. To discretize the surface operator, we can work within the embedding space and use the meshless finite difference approach (Yao et al., 2010; Zhang et al., 2015) to approximate the differential operator. It is shown in (Cheung et al., 2015) that combining the ideas of closest point and meshless methods can handle PDEs on surfaces with corners. Besides of the closest point method, another meshless approach is to directly project the differential operators onto the surface, (Fuselier and Wright, 2013). As all other meshless methods, this projection method does not require any structure for the point distribution in the discretization. Embedding conditions in the closest point approach is replaced by projection operator $I - nn^T$ arisen naturally from the definitions of surface differential operators using the normal $n$ of the surface. Via the meshless interpolant, some generalized finite difference discretization can be obtained.

The current situation of discretizing differential operators on manifolds is rather similar to its $\mathbb{R}^d$ counterpart. By combining surface projections with the RBF interpolant and its derivatives carefully, it is possible to discretize the surface gradient and Laplace-Beltrami operator on a smooth surface with full convergence theories (Fuselier and Wright, 2013; Fuselier and Wright, 2012). Having the RBF interpolant as the key player, the sets of trial centers and collocations are tightly tie together. When the solution and/or the surface changes rapidly in some small region, it makes sense to add more collocation points where in such region to better capture information. One can expect problems of ill conditioning on $\mathbb{R}^d$ reappear on surface. In any symmetric settings, this means adding more trial enters in the region and, potentially if not for sure, numerical instability follows.

In contrast, the unsymmetric strong-form collocation method, a.k.a. the Kansa method, that is already popular for solving PDEs of various kinds in
allows the sets of collocation points and trial centers to be different. The Kansa method is simple to implement which is one of the many reasons for its popularity. It handles scattered data and time-varying discretization with ease. Because of its high flexibility, the number of successful applications of the Kansa method has grown dramatically since the method was proposed in 1990. Theories of the Kansa method are rather limited. However, one certainty is that its original exactly-determined form cannot even guarantee solvability. Yet, this does not make researchers abandon the Kansa method. Alternatively, many variations of modified Kansa methods and rule-of-thumbs have been suggested and numerically studied. It is obvious that the theoretical development does not measure up to the popularity of the Kansa method. In 2006 (Ling et al., 2006), we proved how the Kansa method should be tweaked so that one can ensure solvability. Later, we proved the convergence of an over-determined Kansa-type formulation in maximum norm (Ling and Schaback, 2008). This theory, however, requires solving the system with linear programming which makes it impractical for large problems. Recently, we show, in Chapter 4, that a constraint least-squares Kansa method and weighted least squares Kansa method for general second order elliptic problems with Dirichlet boundary conditions and show that, with certain boundary smoothness and collocation denseness assumptions, such an approach converges at optimal rate, viz. the same convergence rate as in interpolation problems.

In this paper, we aim to take a step forward by applying and analysing the Kansa method on surfaces.

### 4.2 Kansa methods on smooth surface

To get the Kansa formulation working on surface, we take a detour to the finite difference based closest point method by Ruuth et al. (Ruuth and Merriman, 2008) and a meshless extension orthogonal gradients method by Piret (Piret, 2012) for the Laplace-Beltrami operator on smooth manifold. The key idea
we need from them is the constant-along-normal surface embedding. Let $S$ be a closed surface in $\mathbb{R}^d$ with sufficient smoothness and we consider a general second order elliptic partial differential equation $L_S : H^2(S) \to \mathbb{R}$ in the form of:

$$L_S u_S := -a(x)\nabla_S \cdot \nabla_S u_S + b(x) \cdot \nabla_S u_S + c(x)u_S \quad \text{on } S, \quad (4.1)$$

where $\nabla_S := (I - \mathbf{n}n^T)\nabla_E$ with $E \subset \mathbb{R}^d$ denoting the embedding space. In our context, we assume that the embedding space $E$ is a narrow domain in $\mathbb{R}^d$ containing the surface $S$, which has implication to our main convergence theorem. We also assume that the coefficients in (4.1) are well-behaved and bounded. Since $L_S$ consists of two types of differential operators on surfaces, it suffices to consider the embedding for Laplace-Beltrami operator $\Delta_S = \nabla_S \cdot \nabla_S$ and surface gradient operator $\nabla_S$.

### 4.2.1 Laplace Beltrami operator

Let $S$ be a smooth surface in $\mathbb{R}^d$ with codimension one. Let $\nabla_\Omega$ and $\Delta_\Omega$ be the usual Euclidean gradient and Laplacian operators defined in $\Omega \subset \mathbb{R}^d$, respectively. The surface gradient operator on $S$ is defined as

$$\nabla_S := (I - \mathbf{n}n^T)\nabla_\Omega, \quad (4.2)$$

where $\mathbf{n}$ is the unit outward normal vector to the surface $S$ and $I$ is the identity operator. We can see that the surface gradient $\nabla_S u$ coincide with the usual gradient $\nabla_\Omega u$ for any function $u$ satisfy the embedding condition $\partial_n u = n^T \nabla_\Omega u = 0$ on $S$.

The Laplace-Belratmi operator, a.k.a. the surface Laplacian operator, is defined as

$$\Delta_S u := \nabla_S \cdot \nabla_S u = (I - \mathbf{n}\mathbf{n}^T)\nabla_\Omega \cdot (I - \mathbf{n}\mathbf{n}^T)\nabla_\Omega u$$

$$= \Delta_\Omega u - (\mathbf{n}\mathbf{n}^T \nabla_\Omega) \cdot \nabla_\Omega u - (I - \mathbf{n}\mathbf{n}^T)\nabla_\Omega \cdot (\mathbf{n}\mathbf{n}^T \nabla_\Omega u). \quad (4.3)$$
In this case, the Euclidean Laplacian will coincide with the Laplace-Beltrami operator for all \( x \in S \) if the last two terms of (4.3) vanish.

And, we have the following results:

**Lemma 21** (Laplace-Beltrami operator). Let \( S \) in \( \mathbb{R}^d \) be a smooth surface of codimension one with well-defined normal everywhere. Then the surface Laplacian can be written as

\[
\Delta_S u = \Delta_\Omega u - n^T J(\nabla_\Omega u) n - ((I - nn^T)\nabla_\Omega \cdot n)n\nabla_\Omega u,
\]

where \( J(u) \) is the Jacobian matrix of \( u \).

**Proof:** From the definition of surface Laplacian (4.3), it suffices to show that \((nn^T \nabla_\Omega) \cdot \nabla_\Omega u = n^T J(\nabla_\Omega u)n\) and \((I - nn^T)\nabla_\Omega \cdot (nn^T \nabla_\Omega u)\). For the first part, it is easy to verify by the property of trace that

\[
(nn^T \nabla_\Omega) \cdot \nabla_\Omega u = \text{Trace}(J(\nabla_\Omega u)nn^T) = n^T J(\nabla_\Omega u)n.
\]

For the second part, let us consider

\[
(I - nn^T)\nabla_\Omega \cdot (nn^T \nabla_\Omega u) = \text{Trace}(J(nn^T \nabla_\Omega u)(I - nn^T)) = \text{Trace}(J(n)(I - nn^T)n^T \nabla_\Omega u + \text{Trace}(nJ(n^T \nabla_\Omega u)(I - nn^T))) = \text{Trace}(J(n)(I - nn^T)n^T \nabla_\Omega u + \text{Trace}(nJ(n^T \nabla_\Omega u)(I - nn^T)).
\]

□

Once we established Lemma 21, it is ready to simplify the embedding condition for Laplace-Beltrami operator as follows:

**Lemma 22** (Embedding Conditions). Let \( u_S \) be in \( H^2(S) \) defined on a smooth surface \( S \) with well-defined normal everywhere. Let \( u_\Omega \) in \( H^2(\Omega) \), with \( u_\Omega|_S = u_S \), be an extension of \( u_S \) satisfying embedding conditions:

\[
\partial_n u_\Omega = n^T \nabla_\Omega u_\Omega = 0,
\]

(4.4)
and
\[ \partial_n^{(2)} u_\Omega = n^T J(\nabla u_\Omega) n = 0, \]  
(4.5)
for all \( x \in S \). Then, for any differential operator in the form of (4.1)
\[ \mathcal{L}_\Omega u_\Omega = \mathcal{L}_S u_S, \]
everywhere on the surface \( S \).

**Proof:** Lemma 22 follows immediately from Lemma 21. \( \square \)

In (Piret, 2012), the author imposed an embedding condition which involves taking differentiation of the normal vector field of the surface. He has studied the convergence of partial differential equation on sphere. In this paper, with the help of Lemma 21, we impose two embedding conditions which does not involve any derivative of the normal vector field. Moreover, we will provide convergence tests for sphere, ellipsoid and torus.

Let \( \varepsilon_{cp} \), that depends on \( S \), denotes the largest value so that the \( cp \) mapping is well-defined in \( \Omega_\varepsilon \) for all \( \varepsilon \leq \varepsilon_{cp} \). For any smooth surface \( S \subset \mathbb{R}^d \) and any \( \varepsilon < \min\{1, \varepsilon_{cp}\} \), we define the embedding domain by
\[ \Omega_\varepsilon := \left\{ x \in \mathbb{R}^d : \inf_{p \in S} |x - p| < \varepsilon \right\}. \]  
(4.6)

With the embedding conditions (4.4) and (4.5), we can recast surface PDEs to a form very similar to usual PDEs on bounded domain, i.e.,
\[ \mathcal{L}_S u_S = f \quad \text{on} \quad S \subset \Omega_\varepsilon, \quad \Leftrightarrow \quad \begin{cases} \mathcal{L}_{\Omega_\varepsilon} u_{\Omega_\varepsilon} = f \quad \text{in} \quad \Omega_\varepsilon \subset \mathbb{R}^d, \\ \partial_n u_\Omega = \partial_n^{(2)} u_\Omega = 0 \quad \text{on} \quad S. \end{cases} \]  
(4.7)

We denote the exact solution in (4.7) as \( u^*_S \) and \( u^*_{\Omega_\varepsilon} \), respectively. After finding \( u_{\Omega_\varepsilon} \), the solution of the surface PDE is given by restriction \( u^*_S = u^*_{\Omega_\varepsilon}|_S \).

### 4.2.2 Least squares Kansa method for surface PDEs

The Kansa method is our method of choice to solve the elliptic problem (4.7) for \( u_\Omega \). In order to analyze the convergence of the approximation in the Hilbert space \( H^m(\Omega) \), let \( \Phi \) be a symmetric positive definite kernel \( \Phi : \mathbb{R}^d \to \mathbb{R} \) that
have a positive, algebraically decaying Fourier transform. More precisely, we assume the Fourier transform of $\Phi$ satisfies

$$c_1(1 + |\omega|^2)^{-m} \leq \hat{\Phi}(\omega) \leq c_2(1 + |\omega|^2)^{-m},$$  \hspace{1cm} (4.8)$$

for some positive constant $c_1, c_2 > 0$ and $m > d/2$. Then, the native space $N_\Phi(\Omega)$ associated to this kernel $\Phi$ is identical to the Sobolev space (Wendland, 2004)

$$H^m(\mathbb{R}^d) := \{ u \in L_2(\mathbb{R}^d) : \hat{\tilde{f}}(\cdot)(1 + |\cdot|^2)^{m/2} \in L_2(\mathbb{R}^d) \}. \hspace{1cm} (4.9)$$

Moreover, the native space norm

$$\|u\|_{N_\Phi}^2 := \int_{\mathbb{R}^d} \frac{|\hat{u}(\omega)|^2}{\hat{\Phi}(\omega)} d\omega$$

is equivalent to the Sobolev norm

$$\|u\|_{H^m(\mathbb{R}^d)}^2 := \|\hat{\tilde{f}}(\cdot)(1 + |\cdot|^2)^{m/2}\|_{L_2(\mathbb{R}^d)}.$$  

Let $Z$ be a discrete set of $n_Z$ trial centers in the (very narrow) embedding space $\Omega_\varepsilon \supset S$. The finite dimensional trial space is defined as

$$U_{Z,\Phi,\Omega_\varepsilon} := \text{span}\{\Phi(\cdot - z_j) : z_j \in Z\} \subset N_\Phi(\Omega_\varepsilon). \hspace{1cm} (4.10)$$

Assuming the solution $u_{\Omega_\varepsilon}^*$ is in $N_\Phi(\Omega_\varepsilon)$, we look for approximations of $u_{\Omega_\varepsilon}^*$ from the trial space $U_Z$ in the form of

$$u_Z(x) = \sum_{z_j \in Z} \lambda_j \Phi(x - z_j) \in U_{Z,\Phi,\Omega_\varepsilon}. \hspace{1cm} (4.11)$$

In order to measure the denseness of a data set, say $Z$, the mesh norm and the separation distance are defined as

$$h_{Z,\Omega_\varepsilon} := \sup_{\xi \in \Omega_\varepsilon} \min_{z \in Z} |\xi - z|_2 \quad \text{and} \quad q_{Z,\Omega_\varepsilon} := \frac{1}{2} \min_{z_i, z_j \in Z, i \neq j} |z_i - z_j|_2$$

and, on surfaces,

$$h_{Z,S} := \sup_{\xi \in \Omega_\varepsilon} \min_{z \in Z} \text{dist}(\xi, z) \quad \text{and} \quad q_{Z,S} := \frac{1}{2} \min_{z_i, z_j \in Z, i \neq j} \text{dist}(z_i, z_j),$$
where \( | \cdot |_2 \) denotes the standard Euclidean norm on \( \mathbb{R}^d \) and \( \text{dist} \) denotes the shortest distance along the surface \( S \), respectively.

The mesh norm and the separation distance are fundamental gradients for the error and stability analysis. Let us assume that the discrete set \( Z \) is dense enough so that all the theories can be applied. Assume further that the discrete sets are quasi-uniform, i.e., there exists a constant \( \sigma_X > 1 \) such that

\[
\sigma_X^{-1} q_X \leq h_X \leq \sigma_X q_X, \quad X \in \{X, Z\}.
\] (4.12)

In the discretization of the embedded problem (4.7), there are two major components in the discretization error, namely, \textit{approximation error} and \textit{embedding error}. To impose strong-form collocation conditions, let \( X \) a discrete sets of \( n_X \) collocation points in \( S \). This set of collocation point has its own responsibility in the discretization. On one hand, \( X \) is used to collocate the partial differential equation \( L_{\Omega_\varepsilon} u_{\Omega_\varepsilon} = f \) and hopefully keep the residual \( \| L_{\Omega_\varepsilon} u_{\Omega_\varepsilon} - f \| \) small at \( X \) and in \( \Omega_\varepsilon \) with respect to some norms. On the other hand, \( X \) will also be used to discretely enforce the embedding conditions (4.4). Since our objective is to solve the solution \( u_S \) of the surface PDE instead of \( u_{\Omega_\varepsilon} \) in \( \Omega_\varepsilon \), any error in the embedding conditions will induce some error \( \| L_{\Omega_\varepsilon} u_{\Omega_\varepsilon} - L_{S} u_S \| \), which should also be minimized. Generally speaking, for our proposed least square Kansa methods on surface, the set \( X \) is used to control both the performance of approximating the PDE and approximating the embedding condition.

For any discrete set of points \( X \), we define the discrete norm

\[
\| u \|_A := \left( \sum_{x_i \in A} |u(x_i)|^2 \right)^{1/2} \quad \text{and} \quad \| u \|_{k,A} := \left( \sum_{|\alpha| \leq k} \| D^\alpha u \|_A^2 \right)^{1/2}.
\] (4.13)

Then, the \textit{least square Kansa approximation} to \( u_S^* \) is defined by

\[
u_Z := \arg \min_{v \in U_{S, \varepsilon}} \| L_{\Omega} v - f \|_X^2 + \| \partial_n v \|_X^2 + \| \partial_n^{(2)} v \|_X^2,
\] (4.14)

where \( \Omega_\varepsilon \) is defined as in (4.6). In the minimization problem (4.14), it is trivial to see that the former part is for the approximation of the partial differential
equation while the latter part is for the embedding condition. Moreover, the weighting $\varepsilon$ in the minimization problem (4.14) is used to balance the weight of approximation of the partial differential equation and the approximation of the embedding condition.

For $n_Z = 3n_X$, we have an exactly determined system, which is the formulation found in Piret (Piret, 2012), and the weighting becomes irrelevant. If $n_Z \leq 3n_X$, we have an over-determined setting and we seek for the least-squares solution $\lambda = \{\lambda_1, \ldots, \lambda_{n_Z}\}$ from the following $3n_X$-by-$n_Z$ linear system:

$$\sum_{z_j \in Z} \lambda_j \mathcal{L}_{\Omega_{\varepsilon}} \Phi(x_i - z_j) = f(x_i), \quad x_i \in X \quad (4.15)$$

$$\sum_{z_j \in Z} \lambda_j \partial_n \Phi(x_i - z_j) = 0, \quad x_i \in X \quad (4.16)$$

$$\sum_{z_j \in Z} \lambda_j \partial_n^{(2)} \Phi(x_i - z_j) = 0, \quad x_i \in X. \quad (4.17)$$

The approximation and embedding errors behave differently. It would be more natural to consider these errors separately to yield an optimal weight in order to balance two errors to obtain a good convergence; see Section 4.3 for details.

We will prove the following theorem in the coming section. The least-squares Kansa solution of the boundary value problem (4.7) is convergent.

**Theorem 23.** Let $S$ be a closed $C^m$–surface in $\mathbb{R}^d$, for $d \geq 2$, with codimension one. For any $\varepsilon = \min\{1, \varepsilon_{cp}\}$, let $\Omega_{\varepsilon} \subset \mathbb{R}^d$ be the embedding space such that defined as (4.6). Let $u^*_S \in H^m(S)$ and $u^*_\Omega \in H^m(\Omega_{\varepsilon})$ be the exact solutions to the problems in (4.7) respectively for some integer $m > 3 + d/2$. Let $\Phi$ be a reproducing kernel of $H^m(\Omega_{\varepsilon})$ and let the trial space space $U_Z \subset H^m(\Omega_{\varepsilon})$ of $\Phi$ on $Z$ be defined as (4.10) for some sufficiently dense quasi-uniform sets of trial centers $Z$ such that $C_{\varepsilon}^3 \leq h_{Z,\Omega_{\varepsilon}}$ is satisfied for some constant $C$ depending on $\Omega_{\varepsilon}$ and $\Phi$. Let $X$ be some quasi-uniform set of sufficiently dense discrete collocation points on $S$ such that their fill distances asymptotically. Then the least square Kansa solution $u_Z \in U_Z$ defined by (4.14) satisfies the following
error estimate:
\[
\|u^*_S - u_Z|S\|_{L^2(S)} \leq C_{S, \mathcal{L}_d, \Omega, \Phi, \sigma_X} \left( h_{Z \cap S}^{m-2-1/2} + h_X S h_{Z \cap S}^{m-3-1/2} + h_X S h_{Z \cap S}^{m-1/2} \right) \|u^*_S\|_{H^{m-1/2}(S)}.
\]
holds for sufficiently small \(h_{Z, \Omega, \epsilon, \Phi, \sigma_X} \cap S, S + h_X S h_{Z, \Omega, \epsilon, \Phi, \sigma_X} \cap S, S + h_{Z, \Omega, \epsilon, \Phi, \sigma_X} \cap S\) and some constant \(C\) depending on \(L, \Omega, \Phi, \sigma_X\).

4.3 Results relating \(\Omega_\epsilon\) and \(S\).

Let \(S\) in \(\mathbb{R}^d\) be a smooth \(d-1\) dimensional compact embedded sub-manifold of \(\mathbb{R}^d\). Let \(u_S \in H^m(S)\) be defined on \(S\). Let \(cp: \mathbb{R}^d \to S\) be the closest point mapping such that \(cp(x) = \arg\min_{y \in S} |x - y|\) for all \(y \in E\). i.e.

\[
(u_S \circ cp)(x + t\mathbf{n}) = u_S(x) \quad (4.18)
\]
for all \(-\epsilon \leq t \leq \epsilon\) and \(x \in S\). In particularly, \((u_S \circ cp)(x) = u_S(x)\) for all \(x \in S\).

First, we established the relationship between the norm on \(S\) and the norm on \(\Omega_\epsilon\) for our special type of function \(u_S \circ cp\) and special type of domain.

**Lemma 24.** Let \(S\) be a \(d-1\) dimensional twice continuously differentiable closed surface and \(\Omega_\epsilon\) be defined in (4.6). Then, there exists constant \(c\) and \(C\) such that

\[
c\sqrt{\epsilon}\|u_S\|_{H^m(S)} \leq \|u_S \circ cp\|_{H^m(\Omega_\epsilon)} \leq C\sqrt{\epsilon}\|u_S\|_{H^m(S)}.
\]

**Proof:** Let \(S_t = \{x + t\mathbf{n} : x \in S\}\) be a translated surface along the normal vector field, we have

\[
\int_{S_t} [(u_S \circ cp)(x)]^2 ds = \int_S [(u_S \circ cp)(x + t\mathbf{n})]^2 ds = \int_S u_S^2(x) ds.
\]

Let \(\alpha\) be an multi-index such that \(|\alpha| = k\). As long as \(cp \in C^m(\Omega_\epsilon)\), there is a constant \(C\) such that \(|D^\alpha cp| \leq C\). Then by chain rule we have \(|D^\alpha (u_S \circ cp)| \leq \]
\[ C \sum_{|\alpha| \leq k} D^\alpha u_S \circ cp \]
\[ \int_{S_t} [D^\alpha (u_S \circ cp) (x)]^2 ds \leq C \sum_{|\alpha| \leq k} \int_{S_t} [(D^\alpha u_S \circ cp) (x + t n)]^2 ds \]
\[ = C \sum_{|\alpha| \leq k} \int_{S} [D^\alpha u_S (x)]^2 ds \]

Therefore,
\[ \| u_S \circ cp \|^2_{H^m(S)} = \sum_{|\alpha| \leq m} \int_{\Omega_\epsilon} [D^\alpha (u_S \circ cp) (x)]^2 ds \]
\[ = \sum_{|\alpha| \leq m} \int_{-\epsilon}^\epsilon \int_{S_t} [D^\alpha (u_S \circ cp) (x)]^2 ds dt \]
\[ \leq C \sum_{|\alpha| \leq m} \int_{-\epsilon}^\epsilon \int_{S} [D^\alpha u_S (x)]^2 ds dt \]
\[ = \varepsilon C \sum_{|\alpha| \leq m} \int_{S} [D^\alpha u_S (x)]^2 ds \]
\[ = \varepsilon C \| u_S \|^2_{H^m(S)}. \]

And there is another constant \( c \) such that
\[ \| u_S \circ cp \|^2_{H^m(S)} \]
\[ \geq c \sum_{|\alpha| \leq m} \int_{-\epsilon}^\epsilon \int_{S_t} [(D^\alpha u_S \circ cp) (x)]^2 ds dt \]
\[ = c \sum_{|\alpha| \leq m} \int_{-\epsilon}^\epsilon \int_{S} [(D^\alpha u_S) (x)]^2 ds dt \]
\[ = c \varepsilon \int_{-\epsilon}^\epsilon \int_{S} [(D^\alpha u_S) (x)]^2 ds = c \varepsilon \| u_S \|^2_{H^m(S)} \]

i.e., we have
\[ c \sqrt{\varepsilon} \| u_S \|_{H^m(S)} \leq \| u_S \circ cp \|_{H^m(\Omega_\epsilon)} \leq C \sqrt{\varepsilon} \| u_S \|_{H^m(S)}. \]
\[ (4.19) \]

The next Lemma relates the norm on \( S \) and \( \Omega_\epsilon \) for function in the trial space \( U_{Z, \phi, \Omega_\epsilon} \).
Lemma 25. Let $u_Z$ be any function in the trial space $U_{Z,\Phi,\Omega_e}$ and $u$ be any functions in $H^k(\Omega_e)$, $k < m$. If the trial centers $Z$ is quasi-uniformly distributed and satisfy the denseness requirements that $C_{\Omega,\Phi}\varepsilon^{3/2}h_{Z,\Omega_e}^{-(k+1)} < 1/2$, we have

$$\|u_Z\|_{H^k(\Omega_e)} \leq 2\sqrt{\varepsilon}\|u|_S\|_{H^k(S)}, \quad \forall k < m, u_Z \in U_{Z,\Phi,\Omega_e}$$

and

$$\|u\|_{H^k(S)} \leq \frac{1}{\sqrt{\varepsilon}}\|u\|_{H^{k+1}(\Omega_e)}, \quad \forall u \in H^{k+1}(\Omega_e).$$

Proof: Consider

$$\|u\|_{H^k(\Omega_e)}^2 = \sum_{|\alpha| \leq k} \int_{\eta}^{\xi} \int_{S_t} |D^\alpha u(x)|^2 dxdt = \sum_{|\alpha| \leq k} \int_{\eta}^{\xi} \int_{S} |D^\alpha u(x + t\mathbf{n})|^2 dxdt.$$  

(4.22)

By Taylor theorem on $t$, we have, for some $0 < \xi(x) < t$,

$$D^\alpha u(x + t\mathbf{n}) = D^\alpha u(x) + t\partial_n D^\alpha u(x + \xi\mathbf{n}).$$

(4.23)

Taking square on both side, (4.23) becomes

$$(D^\alpha u(x + t\mathbf{n}))^2 = (D^\alpha u(x))^2 + 2tD^\alpha u(x)\partial_n D^\alpha u(x + \xi\mathbf{n}) + t^2(\partial_n D^\alpha u(x + \xi\mathbf{n}))^2$$

$$(D^\alpha u(x))^2 = (D^\alpha u(x + t\mathbf{n}))^2 - 2tD^\alpha u(x)\partial_n D^\alpha u(x + \xi\mathbf{n}) + t^2(\partial_n D^\alpha u(x + \xi\mathbf{n}))^2$$

Substituting back into (4.22), we have

$$\|u\|_{H^k(\Omega_e)}^2 = 2\varepsilon\|u\|_{H^k(S)}^2 + I_1 + I_2,$$

and

$$2\varepsilon\|u\|_{H^k(S)}^2 = \|u\|_{H^k(S)}^2 - I_1 + I_2,$$

where

$$I_1 = 2\sum_{|\alpha| \leq k} \int_{\eta}^{\xi} \int_S tD^\alpha u(x)\partial_n D^\alpha u(x + \xi\mathbf{n}) dsdt;$$

$$I_2 = \sum_{|\alpha| \leq k} \int_{\eta}^{\xi} \int_S t^2(\partial_n D^\alpha u(x + \xi\mathbf{n}))^2 dsdt.$$
Applying Cauchy-Schwarz inequality, the integrals become

\[ I_1 = \int_{-\varepsilon}^{\varepsilon} t dt \sum_{|\alpha| \leq k} \int_{\mathcal{S}} D^\alpha u(x) \partial_\alpha D^\alpha u(x + \xi n) ds = 0, \]

and

\[ I_2 = \int_{-\varepsilon}^{\varepsilon} t^2 dt \sum_{|\alpha| \leq k} \int_{\mathcal{S}} (\partial_\alpha D^\alpha u(x + \xi n))^2 ds dt \]

\[ \leq \frac{2}{3} \varepsilon^3 \sum_{|\alpha| \leq k} \int_{\mathcal{S}} (D^\alpha u(x + \xi n))^2 dx \]

\[ \leq \frac{2}{3} \varepsilon^3 \sum_{|\alpha| \leq k} \int_{-\varepsilon}^{\varepsilon} \int_{\mathcal{S}} (D^\alpha u(x))^2 dx dt = \frac{2}{3} \varepsilon^3 \| u \|^2_{H^{k+1}(\Omega_\varepsilon)}. \]

Therefore, we have

\[ \| u \|^2_{H^k(\Omega_\varepsilon)} \leq 2\varepsilon \| u \|^2_{H^k(\mathcal{S})} + \frac{2}{3} \varepsilon^3 \| u \|^2_{H^{k+1}(\Omega_\varepsilon)}, \]  

(4.24)

and

\[ 2\varepsilon \| u \|^2_{H^k(\mathcal{S})} \leq \| u \|^2_{H^k(\Omega_\varepsilon)} + \frac{2}{3} \varepsilon^3 \| u \|^2_{H^{k+1}(\Omega_\varepsilon)}. \]  

(4.25)

For any \( u_Z \in U_{Z, \Omega_\varepsilon} \), applying inverse inequality the last term of (4.24) and the fact that \( \| u_Z \|_{L^2(\Omega_\varepsilon)} \leq \| u_Z \|_{H^k(\Omega_\varepsilon)} \), we have

\[ \| u_Z \|_{H^k(\Omega_\varepsilon)} \leq \sqrt{2\varepsilon} \| u_Z \|_{H^k(\mathcal{S})}. \]  

(4.26)

as long as the denseness requirement \( C_{\Omega_\varepsilon} \varepsilon^{3/2} h_{Z, \Omega_\varepsilon}^{-(k+1)} < 1/2 \) is satisfied.

On the other hand, for any \( u \in H^k(\Omega_\varepsilon) \), (4.25) becomes

\[ 2\varepsilon \| u \|^2_{H^k(\mathcal{S})} \leq \| u \|^2_{H^k(\Omega_\varepsilon)} + \frac{2}{3} \varepsilon^3 \| u \|^2_{H^{k+1}(\Omega_\varepsilon)} \]

\[ \leq 2\| u \|^2_{H^{k+1}(\Omega_\varepsilon)}, \]

as \( \varepsilon < 1 \). Finally, we have

\[ \| u \|_{H^k(\mathcal{S})} \leq \frac{1}{\sqrt{\varepsilon}} \| u \|_{H^{k+1}(\Omega_\varepsilon)}. \]  

(4.27)

Lemma 26 show the stability of the elliptical problem (4.7).
Lemma 26. Let $S$ be a $d - 1$ dimensional twice continuously differentiable closed surface. Then, we have

$$
\|u_S\|_{H^2(S)} \leq C_S \|\mathcal{L}_{\Omega_e}(u_S \circ cp)|_S\|_{L_2(S)}
$$

for any $u_S \in H^3(S)$.

**Proof:** Let $u_S \in H^m(S)$ and $u_S \circ cp \in H^m(\Omega_\varepsilon)$. Considering the regularity estimate of second elliptic equation with Neumann boundary condition on $\Omega_\varepsilon$, we have

$$
\|u_S \circ cp\|_{H^2(\Omega_\varepsilon)} \leq C_{\Omega_e}(\|\mathcal{L}_{\Omega_e}(u_S \circ cp)\|_{L_2(\Omega_\varepsilon)} + \|\partial_n(u_S \circ cp)\|_{H^{1/2}(\partial \Omega_\varepsilon)}).
$$

By the property of $u_S \circ cp$ is constant along normal direction of $S$, we have

$$
\|\partial_n(u_S \circ cp)\|_{H^{1/2}(\partial \Omega_\varepsilon)} = 0.
$$

Moreover, for any $u \in H^1(\Omega_\varepsilon)$, there exists a constant $C$ such that

$$
\|u\|_{L_2(\Omega_\varepsilon)}^2 = \int_{-\varepsilon}^{\varepsilon} \int_{S} u^2(x)dsdt = \int_{-\varepsilon}^{\varepsilon} \int_{S} u^2(x + t\mathbf{n})dsdt = \int_{-\varepsilon}^{\varepsilon} \int_{S} [u^2(x) + t\partial_n u^2(\xi)]dsdt \leq 2\varepsilon \|u\|_{L_2(S)}^2 + C\varepsilon^2
$$

Therefore, by Lemma 24, we have

$$
\|u_S\|_{H^2(S)} \leq \frac{C}{\sqrt{\varepsilon}} \|u_S \circ cp\|_{H^2(\Omega_\varepsilon)} \leq \frac{C_{\Omega_e}}{\sqrt{\varepsilon}} \|\mathcal{L}(u_S \circ cp)\|_{L_2(\Omega_\varepsilon)} \leq C_{\Omega_e}(\|\mathcal{L}_{\Omega_e}(u_S \circ cp)|_S\|_{L_2(S)} + \sqrt{\varepsilon})
$$

for all $0 < \varepsilon < \varepsilon_{cp}$. Note the constant $C_{\Omega_e}$ depends on some open ball bounding $\Omega_\varepsilon$ in which suitable for both $S$ and $\Omega_\varepsilon$ for $0 < \varepsilon \leq \varepsilon_{cp}$. Hence, $C_{\Omega_e}$ can be replaced by $C_S$ and we have

$$
\|u_S\|_{H^2(S)} \leq C_S(\|\mathcal{L}(u_S \circ cp)|_S\|_{L_2(S)} + \sqrt{\varepsilon})
$$
for all $0 < \varepsilon < \varepsilon_{cp}$. Hence, we have

$$\|u_S\|_{H^2(S)} \leq C_S \|L_{\Omega_{\varepsilon}}(u_S \circ cp)\|_{L^2(S)}.$$ 

Lemma 27 combines an modified trace inequality and the inverse inequality for trial functions. All of these result based on the special type of domains (4.6).

**Lemma 27.** Assume $Z$ is uniformly distributed and satisfy the denseness requirement $C_{\Omega, \phi} \varepsilon^{3/2} h_{Z, \Omega_{\varepsilon}}^{-1} < 1/2$. Let $u_Z$ be any functions in trial space $U_{Z, \phi, \Omega_{\varepsilon}}$. Then

$$\|u_Z\|_{H^3(S)} \leq C_{\Omega_{\varepsilon}, \phi} h_{Z, \Omega_{\varepsilon}}^{-4} \|u_Z\|_{L^2(S)}. \quad (4.28)$$

**Proof:** Let $u_Z \in U_{Z, \phi}$, applying the second part of Lemma 25 and the inverse inequality for the right hand side, we have

$$\|u_Z\|_{H^3(S)} \leq \frac{1}{\sqrt{\varepsilon}} \|u_Z\|_{H^4(\Omega_{\varepsilon})} \quad (4.29)$$

$$\leq \frac{C_{\Omega_{\varepsilon}, \phi}}{\sqrt{\varepsilon}} h_{Z, \Omega_{\varepsilon}}^{-4} \|u_Z\|_{L^2(\Omega_{\varepsilon})}. \quad (4.30)$$

Since $u_Z$ is in $U_{Z, \Omega_{\varepsilon}}$, by the first part of Lemma 25 for quasi-uniformly distributed $Z$ satisfying $C_{\Omega_{\varepsilon}, \phi} \varepsilon^{3/2} h_{Z, \Omega_{\varepsilon}}^{-1} < 1/2$, it becomes,

$$\|u_Z\|_{H^3(S)} \leq C_{\Omega_{\varepsilon}, \phi} h_{Z, \Omega_{\varepsilon}}^{-4} \|u_Z\|_{L^2(S)}. \quad (4.31)$$

**4.3.1 Proof of Theorem 23**

Consider the stability estimate in Lemma 26 and the sampling inequality in (Madych, 2006; Arcangeli et al., 2007; Arcangeli et al., 2012), we have

$$\|u^*_S - u_Z\|_{H^2(S)} \quad (4.32)$$

$$\leq C_S \|L_{\Omega_{\varepsilon}}(u^*_S \circ cp)\|_{S} - L_{\Omega_{\varepsilon}}(u_Z|S \circ cp)\|_{S} \|L_{H^2(S)}$$

$$\leq C_S (h_X-h_{\varepsilon}^{d-1}/2) \|L_{\Omega_{\varepsilon}}(u^*_S \circ cp) - L(u_Z|S \circ cp)\|_{X}. \quad (4.33)$$
In order to establish the stability estimate, let us consider (4.33). Note that
\( L_S u^*_S = L_{\Omega_S} u^*_S \circ cp \) on \( S \) and according to the boundedness of the coefficient of the differential operator \( L \), see (Giesl and Wendland, 2007), we have

\[
C_S h_{X,S} \| L_{\Omega_S} (u^*_S \circ cp) |_S - L_{\Omega_S} (u_Z |_S \circ cp) |_S \|_{H^1(S)}
\]
\[
= C_S h_{X,S} \| L_S u^*_S - L_S u_Z |_S \|_{H^1(S)}
\]
\[
\leq C_S \| u^*_S - u_Z |_S \|_{H^1(S)}
\]
\[
\leq C_S \| u^*_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{H^1(S)}
\]
\[
+ \| u_Z |_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{H^1(S)}
\]
\[
\tag{4.35}
\]
\[
+ \| u_Z |_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{H^1(S)}
\]
\[
\tag{4.36}
\]

The term in (4.35) converges due to the convergence of standard interpolation on surface (Fuselier and Wright, 2012). Hence, we focus on (4.36) in the following.

Let \( \Psi(\cdot,\cdot) := \Phi(\cdot,\cdot)|_{S \times S} \) be the restricted kernel of \( \Phi \), see (Fuselier and Wright, 2012). Denote \( I_{\beta,Z,Z,S,\delta} u^*_S = \sum_{x_j \in Z} \beta_j \Psi(\cdot-x_j) \) as the interpolation of \( u^*_S \) in the trial space \( U_{Z,Z,S,\delta} \). Define \( \bar{\beta} \in \mathbb{R}^{|Z|} \) such that
\[
\bar{\beta}_j := \begin{cases}
\beta_j, & x_j \in Z \cap S \\
0, & x_j \notin Z \cap S.
\end{cases}
\]

Let \( E \) be the extension operator from \( N_{S,\delta} \) to \( N_{\Omega,\delta} \) such that \( \gamma E I_{\beta,Z,Z,S,\delta} u^*_S = I_{\beta,Z,Z,S,\delta} u^*_S \), where \( \gamma \) is the trace operator. Moreover,

\[
E I_{\beta,Z,Z,S,\delta} u^*_S = I_{\beta,Z,Z,S,\delta} u^*_S \in U_{Z,Z,S,\delta}.
\]
\[
\tag{4.37}
\]

Therefore, applying Lemma 27, (4.36) becomes

\[
C_S \| u_Z |_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{H^1(S)}
\]
\[
\leq C_S \| u^*_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{H^1(S)}
\]
\[
\leq C_S \| u^*_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{H^1(S)}
\]
\[
+ \| u_Z |_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{H^1(S)}
\]
\[
\tag{4.38}
\]

Substituting (4.38) back into (4.36), we have

\[
C_S \| L_{\Omega_S} (u^*_S \circ cp) |_S - L_{\Omega_S} (u_Z |_S \circ cp) |_S \|_{H^1(S)}
\]
\[
\leq C_S \| u^*_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{H^1(S)}
\]
\[
+ h_{X,S} h_{Z,\Omega,\delta} \| u^*_S - I_{\beta,Z,Z,S,\delta} u^*_S \|_{L^2(S)}
\]
\[
+ h_{X,S} h_{Z,\Omega,\delta} \| u_Z |_S - u^*_S \|_{L^2(S)}
\]
\[
\tag{4.39}
\]
\[
\tag{4.40}
\]
\[
\tag{4.41}
\]
\[
\tag{4.42}
\]
Apply the error estimate for interpolation (Fuselier and Wright, 2012) on \( S \) that,

\[
\|u^*_S - I_{\beta,x,S,S,\Psi}u^*_S\|_{H^k(S)} \leq C_{S,\Psi}L_{Z,x,S,S}^{-1/2}\|u^*_S\|_{H^{m-1/2}(S)}. \tag{4.43}
\]

for \( k < m \), to (4.40) and (4.41) separately, (4.39) becomes

\[
C_{S,\ell_z}h_{X,S}\|L_{\ell_z}(u^*_S \circ cp)|_S - L_{\ell_z}(u_Z|_S \circ cp)\|_{H^k(S)}
\leq C_{S,\ell_z,\Omega_e,\Phi}(h_{X,S}h_{Z,x,S,S}^{-m-1/2}\|u^*_S\|_{H^{m-1/2}(S)}) \tag{4.44}
\]

\[
+ h_{X,S}h_{Z,x,S,S}^{-1/2}\|u^*_S\|_{H^{m-1/2}(S)} + h_{X,S}h_{Z,x,S,S}^{-1/2}\|u^*_S\|_{H^{m-1/2}(S)} \tag{4.45}
\]

Note that (4.46) is in \( L_z \) norm and (4.32) is in \( H^2 \) norm. But there is lack of theory to bring (4.46) from \( L_z \) norm up to \( H^2 \) norm. So, we over-estimate the \( L^2 \) norm by \( H^2 \) norm in (4.32).

As long as the denseness requirement \( C_{S,\ell_z,\Omega_e,\Phi}h_{X,S}h_{Z,x,S,S}^{-1/2} < 1/2 \) is satisfied, the stability estimate:

\[
\|u^*_S - u_Z|_S\|_{L_z(S)}
\leq C_{S,\ell_z,\Omega_e,\Phi}(h_{X,\Omega_e}^{(d-1)/2}\|L_{\Omega_e}(u^*_S \circ cp) - L_{\Omega_e}(u_Z|_S \circ cp)\|_X \tag{4.47}
\]

\[
+ h_{X,S}h_{Z,x,S,S}^{-m-1/2}\|u^*_S\|_{H^{m-1/2}(S)} + h_{X,S}h_{Z,x,S,S}^{-1/2}\|u^*_S\|_{H^{m-1/2}(S)} \tag{4.48}
\]

It remains to focus on the discrete norm on X in (4.47) numerically. Because we do not want to calculate \( u_X \circ cp \), our objective is to obtain a approximation \( u_Z \) only. We then try to eliminate it in the following. Let us consider inserting \( L_{\Omega_e}u_Z \) into (4.34), we have

\[
\|L_{\Omega_e}(u^*_S \circ cp) - L_{\Omega_e}(u_Z|_S \circ cp)\|_X
\leq \|L_{\Omega_e}(u^*_S \circ cp) - L_{\Omega_e}u_Z\|_X + \|L_{\Omega_e}u_Z - L_{\Omega_e}(u_Z|_S \circ cp)\|_X
\leq \|L_{\Omega_e}(u^*_S \circ cp) - L_{\Omega_e}u_Z\|_X + C_{L_{\Omega_e}}\|u_Z - u_Z|_S \circ cp\|_{2,X} \tag{4.49}
\]

By the fact that \( \partial^k_{x}(u_Z|_S \circ cp)(x) = 0, \ k = 1, 2 \) for all \( x \in S \) and \( X \subset S \), the
last term of (4.49) becomes
\[ \| u_Z - u_Z|S \circ cp \|_{2,X} \]
\[ \leq 0 + \| \partial_n u_Z \|_X + \| \partial_n^{(2)} u_Z \|_X \]
Therefore, (4.49) becomes
\[ \| \mathcal{L}_\Omega (u^*_S \circ cp) - \mathcal{L}_\Omega (u_Z|S \circ cp) \|_X \]
\[ = C_L \left( \| \mathcal{L}_\Omega u_Z - f \|_X + \| \partial_n u_Z \|_X + \| \partial_n^{(2)} u_Z \|_X \right) \quad (4.50) \]
Equation (4.50) follows from the fact that \( \partial_n^{(k)} \mathcal{E} u^*_S = 0, \ k = 1,2 \) on \( S \) and \( J(u) : H^m(\Omega_e) \mapsto \mathbb{R} \) is a functional defined as
\[ J(u) := \| \mathcal{L} u \|_X^2 + \| \partial_n u \|_X^2 + \| \partial_n^{(2)} u \|_X^2. \quad (4.51) \]
So our least squares Kansa solution becomes
\[ u_Z := \arg \min_{v \in U_{Z,\Omega_e}} J(v - u^*_S \circ cp). \quad (4.52) \]
Note that the least square problem (4.14) can be rewrite as the minimization problem of \( J(\cdot - u^*_S \circ cp) \), then the minimizer \( u_Z \in U_{Z,\Omega_e} \) yields
\[ J(u_Z - u^*_S \circ cp) \leq J(I_{\beta,Z,\Omega_e,\Phi} u^*_S - u^*_S \circ cp). \]
Moreover, by the boundedness of the differential operators \( \mathcal{L}_\Omega, \partial_n \) and \( \partial_n^{(2)} \), we have
\[ \| \mathcal{L}_\Omega (u^*_S \circ cp) - \mathcal{L}_\Omega (u_Z|S \circ cp) \|_X \]
\[ \leq C_{\mathcal{L}_\Omega} \| I_{\beta,Z,\Omega_e,\Phi} u^*_S - u^*_S \circ cp \|_{2,X} \]
\[ = C_{\mathcal{L}_\Omega} \| I_{\beta,Z,\Omega_e,\Phi} u^*_S - u^*_S \|_{2,X} \]
\[ \leq C_{\mathcal{L}_\Omega} \sqrt{n} h_X^{(d-1)/2} h_Z^{m-2-1/2} \| u^*_S \|_{H^{m-1/2}(S)} \quad (4.53) \]
Thus, stability (4.47) and consistency (4.53) yield the final error estimate
\[ \| u^*_S - u_Z|S \|_{L_2(S)} \]
\[ \leq C_{S,\mathcal{C}_S,\Omega_e,\Phi} \left( h_X^{(d-1)/2} \sqrt{n} h_X^{d/2} h_Z^{m-2-1/2} \right) \| u^*_S \|_{H^{m-1/2}(S)} \]
In particular, if we assume further that $X$ is quasi-uniformly distributed, then $n_X \sim q_X^{-(d-1)}$ and there exists a constant $\sigma_X$ such that $\rho_{X,S} \leq \sigma_X$. Thus, the error estimate becomes

$$\|u^*_S - u_S\|_{L_2(S)} \leq C_{S,L,S,\Omega,\Phi,\sigma_X} \left( h^{m-2-1/2}_Z + h_{X,S}^m h^{m-3-1/2}_Z + h_{X,S} h^{-4}_Z h^{m-1/2}_Z \right) \|u^*_S\|_{H^{m-1/2}(S)}.$$ 

The localized inverse inequality that we used is for $L_2$ norm. We overestimated the $L_2$ norm by $H^2$ norm in the proof of error estimate. Therefore, we have to impose stronger denseness requirement. The denseness requirement in the theorem require $C_{S,L,S,\Omega,\Phi} h_{X,S} h^{-4}_Z \Omega < 1/2$. \qed

If we have a localized inverse inequality for $H^2$ norm, we will get a weaker result

$$\|u^*_S - u_S\|_{H^2(S)} \leq C_{S,L,S,\Omega,\Phi,\sigma_X} \left( h^{m-2-1/2}_Z + h_{X,S}^m h^{m-3-1/2}_Z + h_{X,S} h^{-2}_Z h^{m-2-1/2}_Z \right) \|u^*_S\|_{H^{m-1/2}(S)}.$$ 

with a weaker denseness requirement $C_{S,L,S,\Omega,\Phi} h_{X,S} h^{-2}_Z \Omega < 1/2$.

In fact, the denseness requirement is much lower than that in the main theorem. Numerics show that it can be relaxed to $h_X = O(h_Z)$.

The $\Omega$ is $\varepsilon$ dependent. Decreasing $\varepsilon$ may result in the blow up of those $\Omega$ dependent constants. Such $\Omega$ dependent constants arise from applying localized inverse inequality. Although we did not show the independence of $\Omega_{\varepsilon}$ for the generic constant, numerics show that the constant does not blow up when we decrease the $\varepsilon$. The independence of $\Omega_{\varepsilon}$ for the generic constant will be handled in the future.
4.4 Numerical demonstration

4.4.1 Convergence studies

In this section, we will provide some numerical demonstration to verify the error estimate as we proved in the previous section. Let \( S \) be a surface in \( \mathbb{R}^3 \) and \( \Omega_\varepsilon \) be the embedding domain in \( \mathbb{R}^3 \) as defined in (4.6). Let \( n(x) \) be the unit normal vector field of \( S \) for all \( x \in S \). Let \( Z_0 \) be a set of \( N \) quasi-uniformly distributed points on the surface \( S \). Let \( Z = \{ z \pm h_{Z,S}n : z \in Z_0 \} \) be the set of trial centres in the embedding domain \( \Omega \). The set of collocation point \( X \) will be selected from \( S \) only. In the following examples, we will use \( h_{Z,S} \approx 1/\sqrt{N} \) as an approximated measure for the mesh norm on \( S \).

To test the numerical order of convergence, we consider solving the modified Helmholtz equation

\[
-\Delta_S u_S + u_S = f, \tag{4.54}
\]

on unit sphere, ellipsoid and torus, respectively. The equation of unit sphere, ellipsoid and torus will be given as

\[
S_{\text{sphere}} = \{ (x, y, z) : x^2 + y^2 + z^2 = 1 \},
\]

\[
S_{\text{ellipsoid}} = \{ (x, y, z) : x^2/1.6^2 + y^2/0.6^2 + z^2/1.4^2 = 1 \}
\]

and

\[
S_{\text{torus}} = \{ (x, y, z) : (1 - \sqrt{x^2 + y^2})^2 + z^2 = 1/9 \},
\]

respectively.

For the case of unit sphere and ellipsoid, we set the analytical solution to be \( u(x, y, z) = xz \) for all \( (x, y, z) \in S \). \( f \) is computed analytically by the definition of Laplace-Beltrami operator: \( f = -(I - nn^T) \nabla \cdot (I - nn^T) \nabla u + u \). For the case of torus, it has a parameterization in the form of

\[
x(\theta, \varphi) = (1 + \frac{1}{3} \cos \theta) \cos \varphi
\]

\[
y(\theta, \varphi) = (1 + \frac{1}{3} \cos \theta) \sin \varphi
\]

\[
z(\theta, \varphi) = \sin \theta.
\]

The analytical solution is set to be \( u(\theta, \varphi) = \frac{1}{3} \sin \theta \) and the Laplace-Beltrami operator of \( u \) is given by \( \Delta_S(\theta, \varphi) = -3 \sin \theta + \frac{\sin \theta \cos \varphi}{1 + \frac{1}{3} \cos \theta} \). Hence, \( f \) can be computed analytically.
Figure 4.1, 4.2 and 4.3 plot the root mean square error for different kernels and different collocation denseness. For the second row, the number of collocation points is equal to the number of trial centers. For the third row, the number of collocation points is two times to that of trial centers. For the fourth row, the number of collocation points is three times to that of trial centers. It is obvious that all of these setting is convergent for all sphere, ellipsoid and torus. However, when $h_Z = h_X$ is used, the rate of convergence is a bit slower than $h_Z = 2h_X$ and $h_Z = 3h_X$. It means that $h_Z = h_X$ is not enough for our case. On the other hand, the order of convergence for $h_Z = 3h_X$ is almost identical to that of $h_Z = 2h_X$. It means that $h_Z = 3h_X$ is actually not necessary. $h_Z = 2h_X$ is good enough for our cases. In Theorem 23, the denseness requirement that $C_{S,\omega,\Phi} h_X h_Z^{-4} < 1/2$ is quite strong at all. Numerical experiments show that this strong condition can be relaxed to $h_Z h_X$ which is more reasonable.

In our numerical experiments, the numerical order of convergence are higher than the one in Theorem 23. For the sphere and the torus, we can see that the order of convergence increase with the smoothness of the Matern kernel. We also plot the error for multiquadric and Gaussian kernel for comparison. The spectral convergence of these two kinds of kernel are also seen.

### 4.4.2 Application to Reaction-Diffusion system on surface

As an application, let us consider the reaction-diffusion system:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \delta_u \Delta_S u + f_u(u, v) \\
\frac{\partial v}{\partial t} &= \delta_v \Delta_S v + f_v(u, v)
\end{align*}
\]

(4.55)

where $f_u(u, v) = a - (b + 1)u + u^2 v$ and $f_v(u, v) = bu - u^2 v$.

Pattern formation on surfaces can be easily obtained by solving the reaction-diffusion system (4.55), (Turk, 1991; Bertalmio et al., 2001; Turing, 1952). To solve this reaction diffusion system, we apply the second order implicit-explicit (IMEX) time stepping scheme (Ascher et al., 1995; Ruuth, 1995). The steady
Figure 4.1: Convergence studies on unit sphere. Up right: number of collocations equals number of trial centres. Bottom left: number of collocations equals two times of trial centres. Bottom right: number of collocations equals three times of trial centres.

Gaussian

MQ

$h_Z = 2h_X$

$h_Z = h_X$

$h_Z = 3h_X$
Figure 4.2: Convergence studies on ellipsoid. Up right: number of collocations equals number of trial centres. Bottom left: number of collocations equals two times of trial centres. Bottom right: number of collocations equals three times of trial centres.
Figure 4.3: Convergence studies on torus. Up right: number of collocations equals number of trial centres. Bottom left: number of collocations equals two times of trial centres. Bottom right: number of collocations equals three times of trial centres.
state solution is obtained for $T = 30$ with $\Delta t = 0.01$. We solve the diffusive term implicitly and the reaction term explicitly. It results to solve a modified Helmholtz equation

$$-\Delta t \Delta_S u^{n+1} + 3u^{n+1} = 4\Delta t f(u^n) - 2\Delta t f(u^{n-1}) + 4u^n - u^{n-1}$$

in each time step.

The initial condition for both $u$ and $v$ are set to uniformly random values between $-0.5$ and $0.5$. The parameters are set to $\delta_v = 10/900$, $a = 3$ and $b = 10.2$.

We consider two type of surface in this simulation. Torus and orthocircle. The torus is identical to that in the previous example. The equation of the orthocircle is given by

$$S_{orthocircle} = \{(x, y, z) : ((x^2 + y^2 - 1)^2 + z^2)((y^2 + z^2 - 1)^2 + x^2)((z^2 + x^2 - 1)^2 + y^2) - \alpha^2(1 + \beta(x^2 + y^2 + z^2))\}$$

with two parameters $\alpha = 0.075$ and $\beta = 3$. Figure 4.4 shows the steady state solution ($T = 30$) for both unit sphere and torus. The pattern shown in 4.4 is similar to that in (Macdonald and Ruuth, 2009; Yang et al., 2004). The left column shows the stripes on the torus and the orthocircle while the right shows the honeycomb.

### 4.4.3 Generalization to open surfaces

In the previous sections, we developed a numerical formulation for solving partial differential equations on closed smooth surfaces. Actually, one can easily extend this idea from closed surface to surfaces with boundary. Let us consider a second order elliptic boundary value problem on a smooth surface with smooth boundary:

$$\begin{cases}
L_S u_S = f & \text{in } S \\
B u_S = g & \text{on } \partial S.
\end{cases} \tag{4.56}$$
Figure 4.4: Turing pattern on sphere and torus. Left: $\delta_u = 5/900$. Right: $\delta_v = 3.8/900$. 
Let \( X \in S \), \( Y \in \partial S \) and \( Z \in \Omega \). A modification of the least square formulation (4.15)-(4.17) is given by

\[
\sum_{z_j \in Z} \lambda_j \mathcal{L}_{\Omega} \Phi(x_i - z_j) = f(x_i), \quad x_i \in X
\]
\[
\sum_{z_j \in Z} \lambda_j \partial_n \Phi(x_i - z_j) = 0, \quad x_i \in X
\]
\[
\sum_{z_j \in Z} \lambda_j \partial^{(2)}_n \Phi(x_i - z_j) = 0, \quad x_i \in X
\]
\[
\sum_{z_j \in Z} \lambda_j B \Phi(x_i - z_j) = g(y_i), \quad y_i \in Y.
\]

The numerical solution to (4.56) is obtained by solving a least square problem:

\[
u_Z := \arg \min_{v \in U_Z, \Phi, \Omega} \| \mathcal{L}_\Omega v - f \|_X^2 + \| \partial_n v \|_X^2 + \| \partial^{(2)}_n v \|_X^2 + \| B v - g \|_Y^2.
\] (4.57)

One may show that there is an analogous error estimate for smooth surface with smooth boundary. It will be handled in the future and we will just show by numerics that the numerical solution is convergent with certain order of convergence.

As an numerical experiment for solving PDEs on surfaces with boundary, let us consider the modified Helmholtz equation with Neumann boundary condition on hemisphere \( S = \{(x, y, z) : x^2 + y^2 + z^2 = 1 \text{ and } z \geq 0\}:

\[
\begin{cases}
-\Delta_S u + u = f & \text{in } S \\
B u = g & \text{on } \partial S,
\end{cases}
\] (4.58)

where \( B u = u \) or \( B u = \partial_n u \). The analytical solution to this problem is set to \( u(x, y, z) = xz \) for \( (x, y, z) \in S \) and \( f \) and \( g \) are computed analytically by definition.

Figure 4.5 investigate the convergence of (4.58) with Dirichlet boundary condition. i.e., \( B u = u = g \) on \( \partial S \). On the other hand, figure 4.6 study the convergence of (4.58) with Neumann boundary condition. i.e., \( B u = \partial_\nu u = g \) on \( \partial S \) where \( \nu = \begin{bmatrix} 0 & 0 & -1 \end{bmatrix}^T \). It is obvious that the numerical solutions converge to the analytical solution for both types of boundary condition. The order of convergence is not as fast as that for surfaces without boundary. Moreover,
Figure 4.5: Convergence studies on Hemisphere with Dirichlet boundary condition. Up right: number of collocations equals number of trial centres. Bottom left: number of collocations equals two times of trial centres. Bottom right: number of collocations equals three times of trial centres.

it seems that the order of convergence does not increase with the smoothness of the Whittle-Matérn-Sobolev kernels for the case of Neumann boundary condition. But it does increase with the smoothness of the Whittle-Matérn-Sobolev kernels for the case of Dirichlet boundary condition.

To the end of this chapter, we consider solving the reaction-diffusion system on surfaces with boundary. We impose the homogeneous Neumann boundary condition to (4.55) and solve by the least-square formulation (4.57). Similar to the results for surface without boundary. The stripe and honeycomb pattern can be recovered and they are shown in figure 4.7.
Figure 4.6: Convergence studies on Hemisphere with Neumann boundary condition. Up right: number of collocations equals number of trial centres. Bottom left: number of collocations equals two times of trial centres. Bottom right: number of collocations equals three times of trial centres.

Figure 4.7: Turing pattern on hemisphere. Left: $\delta_u = 5/900$. Right: $\delta_v = 3.8/900$. 

4.5 Conclusion

In this Chapter, we use least square Kansa’s method to solve second order elliptic partial differential equation on surface. This method requires imposing two homogeneous embedding condition, namely, first zero normal derivative and second zero normal derivative. This method does not require differentiating the normal vector field. In comparison with the method in Chapter two, that method can be recovered when we discretize two homogeneous embedding conditions with central difference method. Hence, it can be viewed as a low order method to the method discussed in this Chapter. In the convergence proof, we proved that the least square solution of second order elliptic partial differential equation converges to the analytical solution according to the smoothness of the kernel we used. The denseness requirement in the proof is quite strong. However, numerical experiments show that the denseness requirement is actually quite weak. Numeric are also provided to justify the theoretical error estimation. Finally, as an important application to surface PDE, we simulate the Turing pattern on torus and orthocircle. We also consider surface with smooth boundary. We numerically showed that the least-square solution is convergent for this case.
Chapter 5

Conclusion

In conclusion, several numerical methods have been proposed for solving different kinds of PDE problem.

In chapter 2, we introduce the closest point method for solving PDEs on surfaces. For the standard closest point methods with finite difference method, interpolation error will be introduced at each closest point extension. In other words, if we solve the PDEs involving time evolution, interpolation error will be accumulated in each time step of the time discretization. With the help of meshless method, a particular data distribution can avoid such interpolation steps. In fact, the particular $S$-orthogonal data distribution replace the closet point mapping as described in (Ruuth and Merriman, 2008). For solving the embedded PDEs, a localized meshless method RBF-FD is employed to discretize the differential operator. Such localized meshless method can be viewed as the generalized finite difference method. Finite difference weighting is obtained and this weighting solved by RBF-FD has optimal error norm of some native spaces. An a priori error estimate which depends only on the data points and kernel can also be provided to investigate the goodness of such data distribution. Moreover, surfaces with fold as a singularity are also considered. A special strategy for dealing with this kind of folded surface is by splitting the approximated differential operator into two parts. i.e., by the average of two one-sided approximations. In the numerical demonstration, diffusion on some
kind of folded surface including the flat-top sphere and the punch-in sphere has been considered. At the end of chapter 2, application of pattern formation and spiral formation on open surface with triple junction are considered.

In Chapter 3, we investigate the $H^2$ norm convergence of least square Kansa solution of second order elliptic partial differential equation. We prove both error estimates for constraint least-square Kansa method and weighted least-square Kansa method for the solution of general second order elliptic partial differential equation. The error estimate based on the results for those kernel with reproducing kernel Hilbert space $H^m(\Omega)$. In the case of weighted least-square Kansa method, we figure out the weightings for PDE collocation and boundary collocation, respectively. We also proved a $H^2$ norm localized inverse inequality. It helps to prove the stability results of both constraint and weighted least-square solution. We also verify the error estimates by some numerical experiments. It shows that both constraint least-square Kansa method and weighted least-square method converge to the analytical solution as expected.

In Chapter 4, we proved the convergence of solving second order elliptic partial differential equation on smooth surface. Instead of solving partial differential equation on surface, we solve the partial differential equation on its embedding space, which is a subset in its ambient space. To solve partial differential equation in the embedding space, some embedding conditions have to be satisfied. The embedding condition of Laplace-Beltrami operator involve the first normal derivative and the second normal derivative. These two embedding conditions is derivative free while the embedding condition in (Piret, 2012) require to differentiate the normal vector. In Chapter 3, we developed the $H^2$ convergence theory for solving second order elliptic partial differential equation on Euclidean space $\mathbb{R}^d$. We extend this idea to partial differential equation on smooth surface. Hence, we proved the $L_2$ convergence theory for second order elliptic partial differential equation on smooth surface. The denseness requirement for the error estimate is quite strong. However, numeric show that the denseness requirement is not that strong. We verify the error estimate
by numerical experiments on sphere, ellipsoid and torus, we find that the order of convergence is much higher than that predicted in the theory. Finally, as an application to this numerical method to solve second order elliptic partial differential equation on smooth surface, we solve the reaction-diffusion equation by using an implicit-explicit scheme. We handle the diffusion term implicitly and the reaction term explicitly. It results in solving a modified Helmholtz equation for each time steps. At the end of this Chapter, we consider solving PDEs on surface with boundary. Dirichlet and Neumann boundary condition are tested. Numerical solutions to both boundary conditions are convergent numerically.
Bibliography


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Curriculum Vitae

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