

**ANALYSIS OF ITERATIVE METHODS
FOR THE SOLUTION OF
BOUNDARY INTEGRAL EQUATIONS
WITH APPLICATIONS TO
THE HELMHOLTZ PROBLEM**

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by
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This thesis is concerned with the numerical solution of boundary integral equations and the numerical analysis of iterative methods. In the first part, we assume the boundary to be smooth in order to work with compact operators; while in the second part we investigate the problem arising from allowing piecewise smooth boundaries. Although in principle most results of the thesis apply to general problems of reformulating boundary value problems as boundary integral equations and their subsequent numerical solutions, we consider the Helmholtz equation arising from acoustic problems as the main model problem.

In Chapter 1, we present the background material of reformulation of Helmholtz boundary value problems into boundary integral equations by either the indirect potential method or the direct method using integral formulae. The problem of ensuring unique solutions of integral equations for exterior problems is specifically discussed. In Chapter 2, we discuss the useful numerical techniques for solving second kind integral equations. In particular, we highlight the superconvergence properties of iterated projection methods and the important procedure of Nyström interpolation.

In Chapter 3, the multigrid type methods as applied to smooth boundary integral equations are studied. Using the residual correction principle, we are able to propose some robust iterative variants modifying the existing methods to seek efficient solutions. In Chapter 4, we concentrate on the conjugate gradient method and establish its fast convergence as applied to the linear systems arising from general boundary element equations. For boundary integral equations on smooth boundaries we have observed, as the underlying mesh sizes decrease, faster convergence of multigrid type methods and fixed step convergence of the conjugate gradient method.

In the case of non-smooth integral boundaries, we first derive the singular forms of the solution of boundary integral solutions for Dirichlet problems and then discuss the numerical solution in Chapter 5. Iterative methods such as two grid methods and the conjugate gradient method are successfully implemented in Chapter 6 to solve the non-smooth integral equations. The study of two grid methods in a general setting and also much of the results on the conjugate gradient method are new. Chapters 3, 4 and 5 are partially based on publications [4], [5] and [35] respectively.

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Dedicated to

my wife Li Zhuang.

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List of Notation

| | |
|-----------------|----------------------------------------------------------------|
| nD | — n -dimensional |
| \mathcal{B} | — a bounded linear operator |
| c | — a generic constant |
| \mathcal{C} | — a compact operator |
| C^m | — space of m -times continuous and bounded functions |
| $C^{m,\lambda}$ | — space of Hölder continuous and bounded functions |
| C_μ^r | — space of continuous and non-smooth functions |
| D | — the interior domain of a closed boundary S |
| \mathcal{D} | — a bounded linear operator |
| D_+ | — the closed domain $D \cup S$ |
| Δ | — Mellin transform operator |
| E | — the exterior domain of a closed boundary S |
| E_+ | — the exterior domain $E \cup S$ |
| n_q | — outward normal at boundary point $q \in S$ directed into E |
| $G[l]$ | — a grid of N_l nodes usually defined on a non-uniform mesh |
| $G_k(p, q)$ | — the fundamental solution to the Helmholtz equation |
| h_l | — mesh size of the discrete grid $G[l]$ |
| \mathcal{H}_k | — hybrid potential operator |

| | |
|--------------------|--------------------------------------------------------------------------------------------------------------|
| $H_0^{(1)}$ | — first kind Hankel function of order 0 |
| $H_1^{(1)}$ | — first kind Hankel function of order 1 |
| I | — identity matrix |
| \mathcal{I} | — identity operator |
| k | — wave number |
| K | — kernel function of integral operator |
| \mathcal{K} | — linear operator, usually assumed compact (Chapter 2) ; model equation operator, non-compact (Chapter 5) |
| L_k | — single layer potential operator |
| M_k | — double layer potential operator |
| M_k^T | — differential single layer potential operator |
| N_k | — differential double layer potential operator |
| ∇^2 | — Laplace differential operator |
| Ω | — bounded or unbounded domain |
| \mathcal{P}_ℓ | — projection operator |
| Π_n | — a general mesh of $(n+1)$ mesh points |
| R^n | — n D Euclidean space |
| R_n | — a n D rectangle |
| \mathcal{R}_k | — differential hybrid potential operator |
| $S^{n,r}$ | — space of r th order piecewise polynomials over Π_n |
| $S_{u,v}^{n,r}$ | — space of r th order piecewise polynomials(Chapter 5) |
| u, ψ | — solution of integral equations |
| u_n, ψ_n | — approximate solution of integral equations |
| u_n^*, ψ_n^* | — iterated approximate solution of integral equations |

Chapter 1

Boundary Integral Equation

Reformulations

In recent years, boundary element methods (BEM's) have become increasingly acceptable and popular in solving boundary value problems (BVP's) from engineering applications such as applied mechanics, acoustic radiation and scattering, potential flow problems; see [17], [26], [30], [36] and [61]. The research into the solution of boundary integral equations is concerned with the following major aspects of study : (refer to [99] for a more detailed exposition and classification of the main themes)

1. reformulation of boundary value problems into boundary integral equations;
2. solution of boundary integral equations via discretization;
3. numerical solution of the subsequent linear systems.

All above stages will be studied in the thesis. In this chapter, we shall study the stage 1 and present the relevant theoretical results to lay a foundation for

the analysis of the discretization methods in chapters 2 and 5 as well as the analysis of the iterative methods in chapters 3, 4 and 6. In §1.1, we present some theoretical preliminaries for use throughout the thesis. In §1.2, we first derive the Helmholtz equation in the context of acoustic radiation problems and then discuss its solvability. In §1.3, we review the boundary integral equation reformulations of boundary value problems for the Helmholtz equation (on an interior or exterior region). In §1.4, in order to ensure the uniqueness of solutions of integral equations for exterior problems, the methods of Panich [77] and Burton and Miller [29] are adopted. The formulations in this chapter will be valid for both 2D and 3D problems with piecewise smooth boundaries. The very important problem of solvability of solutions of integral equations of the second kind is also discussed. Numerical methods for seeking their solutions are investigated in later chapters.

1.1 Mathematical preliminaries

To formally present boundary integral equation reformulations, we shall need to introduce a few definitions. These include the concept of compact operators used in the well known Riesz-Fredholm theory to establish the solvability of boundary integral equations. For a compact operator, its property of eigenvalue spectrum being (at most) countably infinite and accumulating at one possible point (zero) will be exploited in Chapter 4 in developing the conjugate gradient type methods (CGM's).

Below we shall adopt the usual functional analysis notation. A typical point in R^n is denoted by $x = (x_1, \dots, x_n)$; its norm $|x| = (\sum_{j=1}^n x_j^2)^{1/2}$. $\alpha = (\alpha_1, \dots, \alpha_n)$

denotes an n -tuple of nonnegative integers α_j and x^α denotes the monomial $x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}$, which has the degree $|\alpha| = \sum_{j=1}^n \alpha_j$. Similarly, if $D_j = \partial/\partial x_j$ for $1 \leq j \leq n$, then $D^\alpha = D_1^{\alpha_1} \cdots D_n^{\alpha_n}$ denotes a differential operator of order $|\alpha|$, with $D^{(0, \dots, 0)}\phi = \phi$.

Definition 1.1 (functional spaces of $C^m, C^{m,\lambda}$)

Let Ω be a region in R^n (in the thesis, only $n = 2, 3$ are used). For any non-negative integer m , we define $C^m(\Omega)$ to be the space consisting of all functions ϕ which, together with all their partial derivatives $D^\alpha \phi$ of orders $|\alpha| \leq m$, are bounded and continuous on Ω . If $0 < \lambda \leq 1$, we define $C^{m,\lambda}(\Omega)$ to be the subspace of $C^m(\Omega)$ consisting of those functions ϕ for which, for $|\alpha| = m$, $D^\alpha \phi$ satisfies in Ω a Hölder condition with exponent λ , i.e., there is a constant A such that

$$|D^\alpha \phi(x) - D^\alpha \phi(y)| \leq A|x - y|^\lambda, \quad x, y \in \Omega. \quad \square$$

Definition 1.2 (boundary spaces of $C^m, C^{m,\lambda}$)

Let S be an $(n-1)$ dimensional submanifold of R^n . We call $S \in C^m$, if, for each point $x \in S$, there exists a neighbourhood manifold V_x of x such that the intersection $S \cap V_x$ can be mapped bijectively onto some open domain $U \subset R^n$ and that this mapping $u = f(x)$ satisfies $f \in C^m$. Similarly, we say $S \in C^{m,\lambda}$ if $f \in C^{m,\lambda}$ for $0 < \lambda \leq 1$. □

As a result, if $f \in C^m$ then $f \in C^{m-1,1}$. For simplicity, we denote $C \equiv C^0$ whenever no confusion arises. Define that a subset Θ in a metric space M is *relatively compact* if every sequence in Θ contains a convergent subsequence, and if the limit also lies in Θ , we say Θ is *compact*.

Definition 1.3 (compact operator)

Let X and Y be Banach spaces. A linear operator $\mathcal{K} : X \rightarrow Y$ is called compact if it maps any bounded set in X into a relatively compact set in Y . \square

Recall that the range space of a linear operator $\mathcal{L} : X \rightarrow Y$ is defined by

$$\mathcal{R}(\mathcal{L}) = \{y \mid y = \mathcal{L}x, x \in X\},$$

where X and Y are two Banach spaces. It is easy to show that compact linear operators are bounded and that any linear combination of compact linear operators is compact. Let us formally state some more important results, the proof of which may be found in [11], [36, Ch.1] and [60, Ch.3].

THEOREM 1.4

(1) Let X , Y and Z be Banach spaces and let $\mathcal{K} : X \rightarrow Y$ and $\mathcal{L} : Y \rightarrow Z$ be bounded linear operators. Then the product $\mathcal{K}\mathcal{L}$ is compact if one of the two operators \mathcal{K} or \mathcal{L} is compact.

(2) Let $\mathcal{K} : X \rightarrow Y$ be a bounded linear operator with finite dimensional range $\mathcal{R}(\mathcal{K})$. Then \mathcal{K} is compact.

(3) Let X and Y be two Banach spaces and assume that the sequence $\mathcal{K}_n : X \rightarrow Y$ of compact operators satisfies $\|\mathcal{K}_n - \mathcal{K}\| \rightarrow 0$, $n \rightarrow \infty$, with $\mathcal{K} : X \rightarrow Y$ a linear operator. Then \mathcal{K} is compact.

(4) Let $T, T_n : X \rightarrow X$, $n = 1, 2, \dots$ be bounded linear operators on some Banach space X , and $T_n \rightarrow T$ pointwise i.e., $T_n x \rightarrow T x$, as $n \rightarrow \infty$ for each $x \in X$. Then $\|(T_n - T)\mathcal{K}\| \rightarrow 0$, $n \rightarrow \infty$ for any compact operator $\mathcal{K} : X \rightarrow X$. \square

Let $S \subset \mathbb{R}^m$ (with $m = 2$ or 3) be a Jordan-measurable and compact set (with nonzero measure) and let $C(S)$ be the Banach space of complex-valued continuous functions defined on S with the norm $\|\phi\| = \max_{x \in S} |\phi(x)|$. We now define the important integral operator $\mathcal{K} : C \rightarrow C$ by

$$(\mathcal{K}\phi)(x) = \int_S K(x, y)\phi(y)dy, \quad x \in S, \quad (1.1)$$

where $K(x, y)$ is called the kernel function. If K is well defined and continuous for all $x, y \in S$ and $x \neq y$, and there exist positive constants M and $\alpha \in (0, m - 1]$ such that for all $x, y \in S$, $x \neq y$,

$$|K(x, y)| \leq M|x - y|^{\alpha+1-m}, \quad (1.2)$$

we call both the kernel K and the operator \mathcal{K} weakly singular.

THEOREM 1.5

The integral operator \mathcal{K} with continuous or weakly singular kernel is a compact operator. □

Let us now give a few more definitions which we shall use.

Definition 1.6 (transpose and adjoint operators)

For the integral operator $\mathcal{K} : C \rightarrow C$ as in (1.1),

(1) its transpose $\mathcal{K}^T : C \rightarrow C$ is defined by

$$(\mathcal{K}^T\phi)(x) = \int_S K(y, x)\phi(y)dy, \quad x \in S;$$

(2) its adjoint $\mathcal{K}^ : C \rightarrow C$ is defined by*

$$(\mathcal{K}^*\psi)(x) = \int_S \overline{K(y, x)}\psi(y)dy, \quad x \in S.$$

where \overline{K} denotes the complex conjugate of K . □

Definition 1.7 (null space)

Let X and Y be two Banach spaces and $\mathcal{L} : X \rightarrow Y$ be a linear operator. Then the null space $\mathcal{N}(\mathcal{L})$ of \mathcal{L} in X is defined by

$$\mathcal{N}(\mathcal{L}) = \{\phi \in X \mid \mathcal{L}\phi = 0\}. \quad \square$$

THEOREM 1.8

If \mathcal{K} is compact on a Banach space X , then $\dim(\mathcal{N}(\mathcal{I} - \mathcal{K}))$ is finite. \square

We now give the solvability theorem for a second kind integral equation

$$\phi - \mathcal{K}\phi = f, \quad (1.3)$$

with \mathcal{K} a compact operator as defined in (1.1). The proof of the theorem can be found in [36, Ch.1].

THEOREM 1.9 (Fredholm alternative)

Let $\mathcal{K} : C \rightarrow C$ be compact and \mathcal{K}^* be its adjoint operator as defined in Definition

1.6. Then either

1)

$$\mathcal{N}(\mathcal{I} - \mathcal{K}) = \{0\} \quad \text{and} \quad \mathcal{N}(\mathcal{I} - \mathcal{K}^*) = \{0\}$$

$$\text{and } \mathcal{R}(\mathcal{I} - \mathcal{K}) = \{C\} \quad \text{and} \quad \mathcal{R}(\mathcal{I} - \mathcal{K}^*) = \{C\}$$

or 2)

$$\dim(\mathcal{N}(\mathcal{I} - \mathcal{K})) = \dim(\mathcal{N}(\mathcal{I} - \mathcal{K}^*)) \quad \text{are finite}$$

$$\text{and } \mathcal{R}(\mathcal{I} - \mathcal{K}) = \{h \in C \mid (h, \psi) = 0, \psi \in \mathcal{N}(\mathcal{I} - \mathcal{K}^*)\}$$

$$\text{and } \mathcal{R}(\mathcal{I} - \mathcal{K}^*) = \{g \in C \mid (g, \phi) = 0, \phi \in \mathcal{N}(\mathcal{I} - \mathcal{K})\},$$

where the product of two functions is defined by

$$(g, \phi) = \int_S g(x)\phi(x)dx. \quad \square$$

In general, the null space $\mathcal{N}(\lambda\mathcal{I}-\mathcal{K})$ is defined to be the space of eigenfunctions of operator \mathcal{K} and those values of λ with which such a space is nonempty are called the eigenvalues. The adjoint homogeneous equation of (1.3) is defined by

$$\psi - \mathcal{K}^*\psi = 0, \quad (1.4)$$

where alternatively $\psi \in \mathcal{N}(\mathcal{I} - \mathcal{K}^*)$. Therefore from Theorem 1.9, we make the following conclusions when \mathcal{K} is a compact operator; (refer to [60, Ch.3] and [101, Ch.2]).

- (1) equation (1.3) has a unique solution if and only if (1.4) has only the trivial solutions $\psi(x) \equiv 0$;
- (2) equation (1.3) is solvable only if the function f is orthogonal to any solution of (1.4) i.e. $(f, \psi) = 0$. □

Remark :

Note that Fredholm theories are only applied to integral equations of the second kind with a compact operator; refer to [36] and [101]. Generalization to non-compact operator equations is not yet complete. But for the special case when the non-compactness is due to the non-smooth boundaries, this generalization has been carried out; see [66] and [67] and the references therein for more details. For instance, Theorem 1.9 still holds if \mathcal{K} is the sum of a bounded linear operator with norm less than one and a compact operator. To see this, let

us assume that we have two integral operators \mathcal{K}_1 and \mathcal{K}_2 in space C such that $\|\mathcal{K}_1\|_\infty < 1$ and \mathcal{K}_2 is compact. We want to establish the solvability of equation $(\mathcal{I} - \mathcal{K}_1 - \mathcal{K}_2)\psi = g$. Note that both $(\mathcal{I} - \mathcal{K}_1)$ and $(\mathcal{I} - \mathcal{K}_1)^{-1}$ are bounded and non-zero. From Theorem 1.4(1) we know that the operator $(\mathcal{I} - \mathcal{K}_1)^{-1}\mathcal{K}_2$ is compact. Therefore the solvability of equation

$$[\mathcal{I} - (\mathcal{I} - \mathcal{K}_1)^{-1}\mathcal{K}_2]\psi = (\mathcal{I} - \mathcal{K}_1)^{-1}g,$$

which is equivalent to equation $(\mathcal{I} - \mathcal{K}_1 - \mathcal{K}_2)\psi = g$, follows from Theorem 1.9.

This particular result will be used in Chapter 5.

1.2 Boundary value problems

Firstly, we introduce our boundary value problems, which may arise from some engineering applications. Here we consider the time-harmonic acoustic scattering problem. Suppose an incident sound wave is intercepted by a bounded scatterer. Reflected and diffracted sound waves generated propagate outwards from the scattering region. The propagation can be described by the wave equation

$$\nabla^2 U = \frac{1}{c^2} \frac{\partial^2 U}{\partial t^2} \quad (1.5)$$

where c is the speed of sound in the medium exterior to the scatterer. Here U is a scalar velocity potential related to the particle velocity \underline{u} by

$$\underline{u} = \nabla U$$

and to the sound pressure p by

$$p = -\rho \frac{\partial U}{\partial t},$$

where ρ is the density of the medium. Let us assume that the wavelength of the source radiation is c/f corresponding to a frequency f Hz and that the steady state has been reached so that all waves present have harmonic time dependence of this frequency. Define $\omega = 2\pi f$ to be the angular frequency and $k = \omega/c$ the acoustic wavenumber. Then we can write

$$U(p, t) = \phi(p)e^{-i\omega t} \quad (1.6)$$

where ϕ is a complex function and p is a point in the scattered region. On substituting (1.6) into the wave equation (1.5), we obtain the Helmholtz equation for the unknown function ϕ

$$(\nabla^2 + k^2)\phi = 0. \quad (1.7)$$

(Refer to [7], [10], [26] and [36] for more discussions).

Next we supply equation (1.7) with boundary conditions in order to discuss its solvability. Let D be an open, bounded and simply connected region with closed boundary S and open exterior E , as shown in Fig.1.1. Denote $D_+ = D \cup S$ and $E_+ = E \cup S$. Assume that the boundary S is piecewise smooth *i.e.*,

$$S = S_1 \cup \dots \cup S_J \quad (1.8)$$

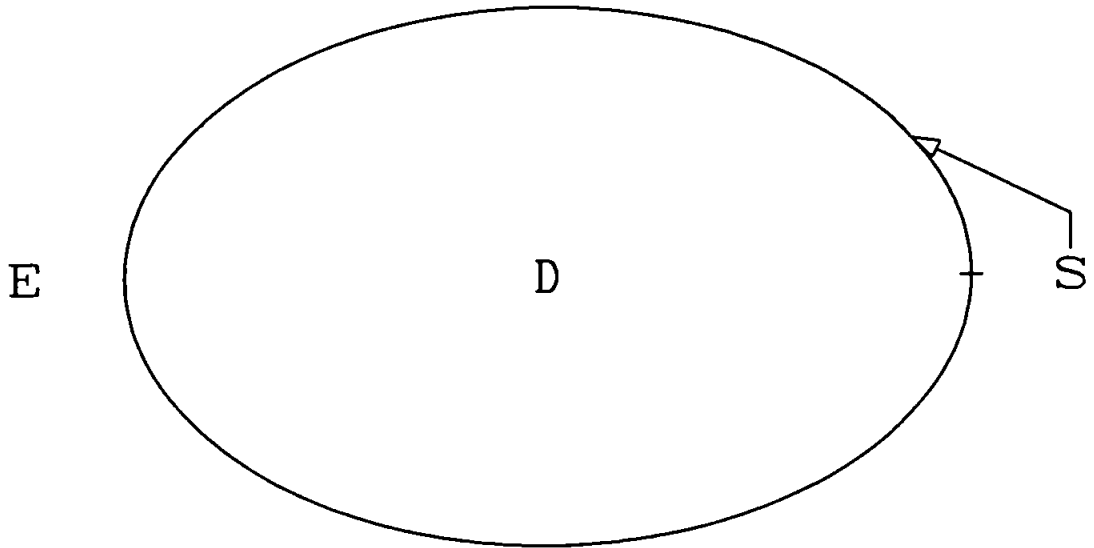
with each S_j of class C^l , $l \geq 2$ and is such that the divergence theorem is valid on D_+ . Then the interior Helmholtz equation is given by

$$\nabla^2 \phi + k^2 \phi = 0, \quad p \in D, \quad (1.9)$$

and the exterior Helmholtz equation by

$$\nabla^2 \phi + k^2 \phi = 0, \quad p \in E, \quad (1.10)$$

Figure 1.1: Boundary S for interior and exterior Helmholtz problems



where $\text{Im}(k) \geq 0$. Typical boundary conditions for both problems on the closed boundary S may be generally represented by

$$a \frac{\partial \phi}{\partial n} + b \phi = f(p), \quad p \in S, \quad (1.11)$$

where $a = 0$ and $b = 1$ define the Dirichlet condition while $a = 1$ and $b = 0$ define the Neumann condition, with n denoting the unit outward normal to S at p directed into E . For exterior problems, we also require the solution to satisfy the so-called Sommerfeld radiation condition, which characterizes the solution behaviour at infinity,

$$\lim_{r \rightarrow \infty} r^\tau \left\{ \frac{\partial \phi}{\partial r} - ik\phi(p) \right\} = 0, \quad \text{with } r = |p|, \quad (1.12)$$

where $\tau = \frac{1}{2}$ for $p \in R^2$ and $\tau = 1$ for $p \in R^3$.

Below we briefly review the theory of uniqueness and existence of the boundary value problems for Helmholtz equations (1.9) and (1.10) with boundary condition (1.11) and also with condition (1.12) for exterior problems. The results are

presented as theorems, the proof of which can be found in [36, Ch.3]. A solution φ to the homogeneous interior Dirichlet problem is that satisfying (1.9) and $\varphi(p) = 0$, $p \in S$ and a solution ψ to the homogeneous interior Neumann problem is that satisfying (1.9) and $\frac{\partial\psi}{\partial n}(p) = 0$, $p \in S$.

THEOREM 1.10 (uniqueness for Helmholtz equations)

- (1) *If $\text{Im}(k) > 0$, then the interior Dirichlet and Neumann problems have at most one solution;*
- (2) *For any complex number k such that $\text{Im}(k) \geq 0$, the exterior Dirichlet and Neumann problems have at most one solution. \square*

THEOREM 1.11 (existence for Helmholtz equations)

- (1) *The interior Dirichlet problem is solvable if and only if*

$$\int_S f \frac{\partial\varphi}{\partial n} dS = 0 \tag{1.13}$$

for all solutions φ to the homogeneous interior Dirichlet problem;

- (2) *The interior Neumann problem is solvable if and only if*

$$\int_S f \psi dS = 0 \tag{1.14}$$

for all solutions ψ to the homogeneous interior Neumann problem;

- (3) *For $\text{Im}(k) \geq 0$, both the exterior Dirichlet and the exterior Neumann problems are uniquely solvable. \square*

In what follows, the free space Green function $G_k(p, q)$, also called the fundamental solution of Helmholtz equation, will play a crucial role. The fundamental

solution G_k satisfies

$$\begin{cases} (\nabla^2 + k^2)G_k(p, q) = \delta(p - q), \\ G_k \text{ satisfying the radiation condition (1.12),} \end{cases} \quad (1.15)$$

where δ is the Dirac delta function and the second requirement is intended for exterior problems. One of such functions has been found to be (refer to [26])

$$G_k(p, q) = \begin{cases} \frac{i}{4} \mathbf{H}_0^{(1)}(kr), & \text{in 2D,} \\ \frac{e^{ikr}}{4\pi r}, & \text{in 3D,} \end{cases} \quad (1.16)$$

where $r = |p - q|$ is the distance between points p and q and $\mathbf{H}_0^{(1)}(x) = J_0(x) + iN_0(x)$ is the Hankel function of the first kind of order zero, with $J_0(x)$ and $N_0(x)$ the zero order Bessel functions of the first kind and of the second kind (also called Neumann's function) respectively. In our analysis for the 2D case, we shall need the following useful properties of Hankel functions :

- (1) $\frac{d\mathbf{H}_0^{(1)}(x)}{dx} = -\mathbf{H}_1^{(1)}(x)$;
- (2) $\frac{d\mathbf{H}_1^{(1)}(x)}{dx} = -\frac{\mathbf{H}_1^{(1)}(x)}{x} + \mathbf{H}_0^{(1)}(x)$;
- (3) $\mathbf{H}_1^{(1)}(x) = J_1(x) + iN_1(x)$;
- (4) $\mathbf{H}_0^{(1)}(x) = \frac{2i}{\pi} \log\left(\frac{x}{2}\right) + O(1)$, as $x \rightarrow 0$;
- (5) $\mathbf{H}_1^{(1)}(x) = -\frac{2i}{\pi} \frac{1}{x} + O(1)$, as $x \rightarrow 0$,

where $J_1(x)$ and $N_1(x)$ are the first order Bessel functions of the first and second kind respectively; refer to [97] for more details. (Note that we may use the **NAG** routines S17AEF, S17AFF, S17ACF and S17ADF to compute functions J_0 , J_1 , N_0 and N_1 numerically).

1.3 Integral equation reformulations for the Helmholtz equation

We now discuss two different but related approaches to reformulate equations (1.9) and (1.10) into boundary integral equations. Such reformulations can transform a boundary value problem defined on a given domain to an equivalent problem (a boundary integral equation) defined only on its boundaries. One of the advantages gained from this process is that the dimensionality of the new problem is consequently reduced by one. For example, a 3D domain problem is reduced to its counterpart on its 2D surface (boundary), while a 2D plane problem is reduced to that defined on its 1D boundary. In particular, for an exterior problem, the integral equation reformulation can advantageously reduce the domain of the problem from the infinite exterior region E to the finite boundary S of the new problem of one dimension less and more importantly ensure that the solutions automatically satisfy the radiation condition (1.12). Then the boundary integral equations may be initially solved to give the boundary information, from which the solution to Helmholtz equation at any point of domain can be evaluated through the integral representation inherent in the formulation.

1.3.1 Helmholtz layer potentials — indirect methods

With the explicit knowledge of fundamental solution $G_k(p, q)$, we can actually construct two independent solutions of Helmholtz equation. They are usually referred to as the layer potentials

$$\text{single-layer } (L_k\sigma)(p) = \int_S \sigma(q)G_k(p, q)dS_q, \quad (1.17)$$

$$\text{double-layer } (M_k\sigma)(p) = \int_S \sigma(q) \frac{\partial G_k}{\partial n_q}(p, q) dS_q, \quad (1.18)$$

where n_q is the outward normal from D directed into E at $q \in S$ and p is any point in Ω (Note that such a normal direction is the same for both the interior and the exterior problems. Refer to [26, p.29]). It is easy to verify by straightforward calculations that for any $p \in \Omega$, both layer potentials $L_k\sigma$ and $M_k\sigma$ satisfy the Helmholtz equation (1.7) and the radiation condition (1.12); see [36, Ch.3]. The function σ is referred to as a boundary density function. By ensuring that the above solutions of the Helmholtz equation satisfy the boundary condition on S , such as (1.11), we can find the appropriate integral equations to be satisfied by the density function σ . By 'indirect methods', we actually emphasize the fact that the unknown density function σ is usually not of immediate physical interest, but is merely an intermediate step in obtaining the appropriate solution of the Helmholtz equation.

To proceed, let us first study the continuity of $L_k\sigma$ and $M_k\sigma$ and their normal derivatives. We only need to look at the problem near S , since these quantities are smooth functions away from the boundary. Let us define two new operators M_k^T and N_k , derivatives of L_k and M_k respectively, which will appear in later formulations :

$$(M_k^T\sigma)(p) = \frac{\partial L_k\sigma}{\partial n_p} = \int_S \sigma(q) \frac{\partial G_k}{\partial n_p}(p, q) dS_q, \quad (1.19)$$

$$(N_k\sigma)(p) = \frac{\partial M_k\sigma}{\partial n_p} = \frac{\partial}{\partial n_p} \int_S \sigma(q) \frac{\partial G_k}{\partial n_q}(p, q) dS_q. \quad (1.20)$$

The compactness of operators L_k , M_k , M_k^T , $N_k - N_0$ as stated in the theorem below follows from [36, Ch.2], where N_0 is the operator N_k with $k = 0$.

THEOREM 1.12 *Assume that boundary $S \in C^2$, then*

(1) operators L_k , M_k , M_k^T and $N_k - N_0$ are compact in C and $C^{0,\lambda}$ for $0 < \lambda < 1$;

(2) $C \xrightarrow{L_k, M_k, M_k^T, N_k - N_0} C^{0,\lambda}$ and $C^{0,\lambda} \xrightarrow{L_k, M_k} C^{1,\lambda}$ for any $0 < \lambda < 1$. \square

The continuity properties of operators L_k , M_k and M_k^T , N_k may be stated, following [17], [26] and [36, Ch.2].

LEMMA 1.13

(1) If σ is continuous, $L_k\sigma$ is also continuous;

(2) If σ is continuous, $M_k\sigma$ and $M_k^T\sigma$ are continuous except on boundary S ,

where

$$\begin{aligned} (M_k\sigma)(p_+) - \frac{\chi(p)}{2}\sigma(p) &= (M_k\sigma)(p) = \frac{\chi(p)}{2}\sigma(p) + (M_k\sigma)(p_-), \\ (M_k^T\sigma)(p_+) + \frac{\chi(p)}{2}\sigma(p) &= (M_k^T\sigma)(p) = -\frac{\chi(p)}{2}\sigma(p) + (M_k^T\sigma)(p_-), \end{aligned}$$

where $\vartheta(p_+)$ denotes the limiting value of a potential function ϑ from the exterior E towards the boundary point $p \in S$ along the normal direction, $\vartheta(p_-)$ similarly denotes the limiting value from the interior towards $p \in S$ along the normal and $\chi(p)\pi$ is the exterior (or interior) angle¹ between the two tangents at a point $p \in S$ for interior (or exterior) problems. Obviously $\chi(p) = 1$ if the boundary S is smooth at p .

(3) If σ is twice continuously differentiable, $N_k\sigma$ is continuous across the boundary S . \square

¹In 3D, this is the solid angle subtended by the domain of the problem. Refer to [6] and [17].

The above lemma facilitates the process of forming equations for the density function σ , by imposing the appropriate boundary conditions. For $p \in \Omega$ (with $\Omega = D$ for the interior and $\Omega = E$ for the exterior problems), we let $\phi(p) = (L_k\sigma)(p)$ and $(M_k\sigma)(p)$ respectively. In order to impose the boundary conditions, we take the limit as p approaches a boundary point along the normal and, using Lemma 1.13, we obtain the following integral equations for various problems :

Interior Dirichlet Problem

$$(L_k\sigma)(p) = f, \quad p \in S, \quad (1.21)$$

$$-\frac{\chi(p)}{2}\sigma(p) + (M_k\sigma)(p) = f, \quad p \in S; \quad (1.22)$$

Interior Neumann Problem

$$\frac{\chi(p)}{2}\sigma(p) + (M_k^T\sigma)(p) = f, \quad p \in S, \quad (1.23)$$

$$(N_k\sigma)(p) = f, \quad p \in S, \quad (1.24)$$

Exterior Dirichlet Problem

$$(L_k\sigma)(p) = f, \quad p \in S, \quad (1.25)$$

$$\frac{\chi(p)}{2}\sigma(p) + (M_k\sigma)(p) = f, \quad p \in S; \quad (1.26)$$

Exterior Neumann Problem

$$-\frac{\chi(p)}{2}\sigma(p) + (M_k^T\sigma)(p) = f, \quad p \in S, \quad (1.27)$$

$$(N_k\sigma)(p) = f, \quad p \in S, \quad (1.28)$$

where the density σ in different equations generally represents different functions.

For each of the above four problems, there is a choice of two integral equations, one being of a first kind and the other of a second kind. The latter formulation

is usually the natural choice mainly because the Fredholm theory for integral equations is about this case for compact operators. (We refer the reader to [21, Ch.1 & 5], [40], [41, Ch.13] and [74, Ch.5] for details of the first kind integral equations).

Unfortunately however none of the above eight integral equations possess unique solutions for all values of k with $\text{Im}(k) \geq 0$. To be more precise, let us define by k_D the set of wavenumbers for which the interior Dirichlet problem has non-trivial solutions and define similarly by k_N the set of wavenumbers for which the interior Neumann problem has non-trivial solutions. It can be shown that both k_D and k_N only contain positive wavenumbers; see [26]. The two sets k_D and k_N are respectively referred to as the eigenvalue spectra of the interior Dirichlet problem and of the interior Neumann problem. For $k \in k_D$, the equations (1.21) and (1.22) for the interior Dirichlet problem and equations (1.27) and (1.28) for the exterior Neumann problem fail to have unique solutions; whilst for $k \in k_N$, the equations (1.23) and (1.24) for the interior Neumann problem and equations (1.25) and (1.26) for the exterior Dirichlet problem fail to have unique solutions; (refer to [26] and [36, Ch.3]).

We call the numbers in the union $k_D \cup k_N$ 'critical wavenumbers'. Then for interior problems, nonuniqueness of integral equations at 'critical wavenumbers' seems to be inherited from boundary value problems², which is a subject outside the scope of our discussion. But for exterior problems, because the solutions of the exterior boundary value problems are unique for all wavenumbers with $\text{Im}(k) \geq 0$, the complication of nonuniqueness for integral equations at 'critical wavenumbers'

²These 'critical wavenumbers' are related to the resonance frequencies of a structure.

($k \in k_D \cup k_N$) arises solely from our attempting an integral representation of the solution rather than from the nature of the problem itself. Methods that are designed to overcome the nonuniqueness difficulty are presented in §1.4.

1.3.2 Helmholtz integral formulae — direct methods

We now introduce alternative integral equation formulations of the Helmholtz equation. By 'direct methods', we mean that integral equations no longer involve an intermediate density function σ but directly relate values of ϕ with $\frac{\partial\phi}{\partial n}$ on the boundary; both quantities usually of physical interests.

Recall Green's second theorem for integration,

$$\int_S (\phi_1 \frac{\partial\phi_2}{\partial n} - \phi_2 \frac{\partial\phi_1}{\partial n}) dS = \int_D (\phi_1 \nabla^2 \phi_2 - \phi_2 \nabla^2 \phi_1) dV, \quad (1.29)$$

where ϕ_1, ϕ_2 are any scalar functions with continuous second derivatives in D_+ and n is the outward unit normal away from D . If both ϕ_1 and ϕ_2 satisfy the Helmholtz equation (1.9) in D , we can obtain from (1.29)

$$\int_S (\phi_1 \frac{\partial\phi_2}{\partial n} - \phi_2 \frac{\partial\phi_1}{\partial n}) dS = 0. \quad (1.30)$$

Here taking $\phi_1 = \phi(q)$ and $\phi_2 = G_k(p, q)$ in the above equation yields

$$\int_S (\phi(q) \frac{\partial G_k}{\partial n_q} - G_k \frac{\partial\phi}{\partial n_q}) dS_q = 0, \quad p \in E, \quad (1.31)$$

i.e., in operator notation,

$$(M_k\phi)(p) - (L_k \frac{\partial\phi}{\partial n})(p) = 0, \quad p \in E. \quad (1.32)$$

Further, the standard Helmholtz integral formulae may be derived (see [26])

for Interior Problems

$$(M_k \phi)(p) - (L_k \frac{\partial \phi}{\partial n})(p) = \begin{cases} -\phi(p), & p \in D, \\ -\frac{\chi(p)}{2} \phi(p), & p \in S, \\ 0, & p \in E. \end{cases} \quad (1.33)$$

On formally differentiating both sides with respect to n_p , we obtain the differentiated Helmholtz formulae

$$(N_k \phi)(p) - (M_k^T \frac{\partial \phi}{\partial n})(p) = \begin{cases} -\frac{\partial \phi}{\partial n_p}(p), & p \in D, \\ -\frac{\chi(p)}{2} \frac{\partial \phi}{\partial n_p}(p), & p \in S, \\ 0, & p \in E. \end{cases} \quad (1.34)$$

Similarly for exterior problems, we may again use Green's second theorem to deduce the Helmholtz formulae. But in this case the Sommerfeld radiation condition will have to be incorporated; refer to [26]. The resulting Helmholtz integral formulae take the form :

for Exterior Problems

$$(M_k \phi)(p) - (L_k \frac{\partial \phi}{\partial n})(p) = \begin{cases} \phi(p), & p \in E, \\ \frac{\chi(p)}{2} \phi(p), & p \in S, \\ 0, & p \in D, \end{cases} \quad (1.35)$$

and by formal differentiation in the direction of n_p

$$(N_k \phi)(p) - (M_k^T \frac{\partial \phi}{\partial n})(p) = \begin{cases} \frac{\partial \phi}{\partial n_p}(p), & p \in E, \\ \frac{\chi(p)}{2} \frac{\partial \phi}{\partial n_p}(p), & p \in S, \\ 0, & p \in D. \end{cases} \quad (1.36)$$

Hence for both interior and exterior problems, values of $\phi(p)$ and $\frac{\partial \phi}{\partial n}(p)$, $p \in S$ will be sufficient to produce the solution $\phi(p')$ at any field point $p' \in \Omega$ (with $\Omega = D$ for interior and $\Omega = E$ for exterior problems). In general therefore the

quantities $\phi(p)$, $\frac{\partial\phi}{\partial n}(p)$, $p \in S$ may be found from the following boundary integral equations

Interior Dirichlet Problem

$$(L_k\mu)(p) = g, \quad g = \frac{\chi(p)}{2}f - (M_k f)(p), \quad p \in S, \quad (1.37)$$

$$-\frac{\chi(p)}{2}\mu(p) + (M_k^T\mu)(p) = g, \quad g = N_k f, \quad p \in S, \quad (1.38)$$

where $\mu = \frac{\partial\phi}{\partial n}$;

Interior Neumann Problem

$$\frac{\chi(p)}{2}\phi(p) + (M_k\phi)(p) = g, \quad g = L_k f, \quad p \in S, \quad (1.39)$$

$$(N_k\phi)(p) = g, \quad g = M_k^T f - \frac{\chi(p)}{2}f, \quad p \in S; \quad (1.40)$$

Exterior Dirichlet Problem

$$(L_k\mu)(p) = g, \quad g = M_k f - \frac{\chi(p)}{2}f, \quad p \in S, \quad (1.41)$$

$$\frac{\chi(p)}{2}\mu(p) + (M_k^T\mu)(p) = g, \quad g = N_k f, \quad p \in S, \quad (1.42)$$

where $\mu = \frac{\partial\phi}{\partial n}$;

Exterior Neumann Problem

$$-\frac{\chi(p)}{2}\phi(p) + (M_k\phi)(p) = g, \quad g = L_k f, \quad p \in S, \quad (1.43)$$

$$(N_k\phi)(p) = g, \quad g = M_k^T f + \frac{\chi(p)}{2}f, \quad p \in S. \quad (1.44)$$

Comparing equations (1.37)-(1.44) with (1.21)-(1.28), we can observe that in each case the corresponding operator equations are identical except for the right hand sides and the exchange of M_k with M_k^T or vice versa³. Furthermore, discussion of

³Since M_k^T is the transpose operator of M_k , therefore if one's homogeneous equation possesses non-trivial solutions, so does the other and vice versa. Refer to (1.4).

uniqueness of solutions for equations (1.37)-(1.44) follows that of (1.21)-(1.28). For interior problems, formulations are unique if $k \notin k_D \cup k_N$ (i.e. if the boundary value problem has a unique solution), giving a choice of integral equations of the first kind and the second kind. For exterior problems, as before in spite of the uniqueness of solutions of the boundary value problem, none of the boundary integral equations (1.41)-(1.44) of the problem are uniquely solvable for all values of k with $\text{Im}(k) \geq 0$. Next we present for exterior problems modified formulations which are uniquely solvable for all wavenumbers.

1.4 Unique formulations for exterior problems

There have been many successful attempts to acquire boundary integral equation formulations for the Helmholtz equation in the exterior domain which possess unique solutions for all wavenumbers $\text{Im}(k) \geq 0$. We refer the reader to [26] and [64] for excellent surveys of these formulations. Theoretically speaking, these modified methods fall into two main categories, either those using a combination of the existing formulations in order to overcome nonuniqueness difficulty i.e. at $k \in k_D \cup k_N$ or those using more sophisticated fundamental solutions to gain uniqueness for all wavenumbers (refer to [36, Ch.3] and [65]). Here we only consider one simple version in the former category, which is perhaps the most widely used for numerical calculations.

Indirect methods

The method we consider here is based on linear combinations of single and double layer potentials in the hope of obtaining unique solutions. For this purpose, we

define the useful hybrid layer potential operator \mathcal{H}_k (refer (1.17) and (1.18))

$$(\mathcal{H}_k\sigma)(p) = (M_k\sigma)(p) - \eta(L_k\sigma)(p), \quad p \in E, \quad (1.45)$$

where η is a complex constant. We also define the differential hybrid layer potential operator by

$$(\mathcal{R}_k\sigma)(p) = (M_k^T\sigma)(p) + \eta(N_k\sigma)(p), \quad p \in E, \quad (1.46)$$

which is similar to the direct differentiation of operator \mathcal{H}_k along the normal direction, where M_k^T , N_k are as defined in (1.19) and (1.20). Now let us make a particular choice for η , which will be very useful later,

$$\eta = i\theta, \quad \theta = \begin{cases} t \text{ s.t. } t \neq 0, tk \geq 0, & \text{if } \text{Im}(k) = 0, \\ 0, & \text{if } \text{Im}(k) > 0. \end{cases} \quad (1.47)$$

(Here note that θ is a real number).

Clearly $\mathcal{H}_k\sigma$ satisfies the Helmholtz equation (1.10) as both $L_k\sigma$ and $M_k\sigma$ do. So we may proceed as in §1.3.1 based on assuming $\phi(p) = (\mathcal{H}_k\sigma)(p)$, $p \in E$ in order to obtain boundary integral equations for the density function σ . To prove the uniqueness of a linear equation, it is sufficient to show that its homogeneous equation has only trivial solutions. Then the following results based on the assumption that $S \in C^2$ can be shown; see [36, Ch.3].

THEOREM 1.14 *Provided that η is chosen as in (1.47),*

(1) *the integral equation of hybrid layer potential for the*

Exterior Dirichlet Problem

$$\frac{\chi(p)}{2}\sigma(p) + (\mathcal{H}_k\sigma)(p) = f, \quad p \in S, \quad (1.48)$$

i.e.

$$\frac{\chi(p)}{2}\sigma(p) + (M_k\sigma)(p) - \eta(L_k\sigma)(p) = f, \quad p \in S, \quad (1.49)$$

is uniquely solvable for all wavenumbers k with $\text{Im}(k) \geq 0$;

(2) the integral equation of differential hybrid layer potential for the

Exterior Neumann Problem

$$-\frac{\chi(p)}{2}\sigma(p) + (\mathcal{R}_k\sigma)(p) = f, \quad p \in S, \quad (1.50)$$

i.e.

$$-\frac{\chi(p)}{2}\sigma(p) + (M_k^T\sigma)(p) + \eta(N_k\sigma)(p) = f, \quad p \in S, \quad (1.51)$$

is uniquely solvable for all wavenumbers k with $\text{Im}(k) \geq 0$. \square

Direct methods

For simplicity, let us define the transposed operators of \mathcal{H}_k and \mathcal{R}_k respectively by

$$\mathcal{H}_k^T\sigma \equiv M_k^T\sigma - \eta L_k\sigma, \quad (1.52)$$

$$\mathcal{R}_k^T\sigma \equiv M_k\sigma + \eta N_k\sigma. \quad (1.53)$$

Recall from §1.3.2 that for each boundary condition we obtained two boundary integral equations. Based on taking linear combinations of these two equations, we obtain the direct methods so that the operator of the new boundary integral equation is either \mathcal{H}_k^T or \mathcal{R}_k^T . In particular, we may take linear combinations of (1.41) and (1.42) for Dirichlet and (1.43) and (1.44) for Neumann boundary conditions respectively. Further, [36, Ch.3] has proved the following results concerning the so-called Burton and Miller approach by assuming $S \in C^2$; see also [29] and [69].

THEOREM 1.15 *Provided that η is chosen as in (1.47),*

(1) *the following direct integral equation formulation for the*

Exterior Dirichlet Problem

$$\frac{\chi(p)}{2}\mu(p) + (\mathcal{H}_k^T \mu)(p) = g, \quad p \in S, \quad (1.54)$$

i.e.

$$\frac{\chi(p)}{2}\mu(p) + (M_k^T \mu)(p) - \eta(L_k \mu)(p) = g, \quad p \in S. \quad (1.55)$$

is uniquely solvable for all wavenumbers k with $\text{Im}(k) \geq 0$, where $\mu = \frac{\partial \phi}{\partial n}$ and $g = (N_k \phi)(p) - \eta((M_k \phi)(p) - \frac{\chi(p)}{2}\phi(p))$;

(2) *the following direct integral equation formulation for the*

Exterior Neumann Problem

$$-\frac{\chi(p)}{2}\phi(p) + (\mathcal{R}_k^T \phi)(p) = g, \quad p \in S, \quad (1.56)$$

i.e.

$$-\frac{\chi(p)}{2}\phi(p) + (M_k \phi)(p) + \eta(N_k \phi)(p) = g, \quad p \in S, \quad (1.57)$$

is uniquely solvable for all wavenumbers k with $\text{Im}(k) \geq 0$, where $g = \frac{\chi(p)}{2}\mu(p) + (L_k \mu)(p) + (M_k^T \mu)(p)$, $\mu = \frac{\partial \phi}{\partial n}$. □

Now we remark that there is little to choose from between an indirect and a direct method. As stated before, the direct methods lead to unknowns that are more meaningful physically. In some practical situations, values of ϕ and $\frac{\partial \phi}{\partial n}$ on the boundary S are of primary importance so the direct method becomes the natural choice. We can also observe that for either boundary conditions (Dirichlet or Neumann) an indirect method leads to equations with simpler right hand sides that are easier computationally. If boundary S is not globally smooth

e.g. piecewise smooth as given in (1.8), then Theorems 1.14 and 1.15 will still be valid; (see [17], [57], [66], [67] and [98] for more details).

Optimal coupling parameter η

As discussed, any choice that satisfies (1.47) can theoretically ensure that integral operators $[\frac{x(p)}{2} + \mathcal{H}_k]$, $[\frac{x(p)}{2} + \mathcal{H}_k^T]$, $[-\frac{x(p)}{2} + \mathcal{R}_k]$ and $[-\frac{x(p)}{2} + \mathcal{R}_k^T]$ are non-singular, hence leading to unique solutions. However the integral equations with such operators can still be ill-conditioned, even though they are theoretically non-singular. For example, the simple choice $\eta = i$ may not be appropriate for all values of k . Therefore the minimization (or 'almost minimization') of condition numbers of these operators is of prime importance.

We now briefly discuss the appropriate choice of the coupling parameter η in order to minimize the condition number of the integral operators. This would require the calculation of the condition numbers of relevant integral operators, which is in general not possible. However for simple integral boundaries, we may only require the computation of the eigenvalues of individual operators such as L_k , M_k , M_k^T and N_k to find their condition numbers, which are often possible to be evaluated analytically. Any results so obtained may be hoped to give some guidance for general cases.

To gain some insight into the problem, [3] and [68] consider the special case when the boundary S is either a unit circle in 2D or a unit sphere in 3D. They concluded that, for a unit sphere in 3D, the almost optimal choice is, for Dirichlet boundary condition, $\eta = \max(1/2, k)i$ or, for Neumann boundary condition, $\eta = ki$ and for both Dirichlet and Neumann boundary conditions on an unit circle in

2D,

$$\eta = \begin{cases} i/\sqrt{\pi^2 + 4(\log \frac{k}{2} + C)^2}, & \text{for small } k, \\ ki/2, & \text{for large } k, \end{cases}$$

where $C \approx 0.5772$ is the Euler constant.

One last interesting point is that the coupling parameter in (1.52) and (1.53) can be made variable *i.e.* $\eta = \eta(p)$, $p \in S$ and $\eta(p)$ is chosen to be a piecewise function on S . For example we may allow $\eta(p) = 0$ on parts of S . This may help saving computational work as well as keeping uniqueness; see [56] for some experiments. But the theoretical analysis remains to be established.

Regularization for singular integral equations

Note that the operator N_k defined in (1.20) is hyper singular, so its existence can only be understood after some transformation in the sense of Cauchy principal value; refer [26]. Although direct solution of integral equations involving N_k has been attempted in [73], it is however possible to regularize the equations so that all operators are compact. In fact, regularization technique is a very common approach in solving Cauchy singular integral equations; refer to [45] and the references therein for more details. Without loss of generality, let us consider only the equation (1.57) and assume that $S \in C^2$ *i.e.* $\chi(p) = 1$. Using the following two facts (a) $N_k - N_0$ is compact (see Theorem 1.12); (b) the identity is true (see [26])

$$L_0 N_0 = (M_0 - \frac{1}{2}I)(M_0 + \frac{1}{2}I), \quad (1.58)$$

we can obtain, by premultiplying (1.44) by L_0 before coupling with (1.43), the following second kind boundary integral equation

$$-\frac{\phi}{2} + M_k \phi + \eta [L_0(N_k - N_0) + M_0^2 - \frac{I}{4}] \phi = g, \quad (1.59)$$

with $g = [L_k + \eta L_0(\frac{I}{2} + M_k^T)] \frac{\partial \phi}{\partial n}$. Now all integral operators are compact on C and $C^{0,\lambda}$ $0 < \lambda < 1$. Therefore equation (1.59) may be represented by (1.3).

Up till now, we have shown that boundary value problems (§1.2) may be reformulated into integral equations of the second kind, characterized by (1.3) *i.e.*

$$\phi - \mathcal{K}\phi = f, \quad p \in S, \quad (1.60)$$

where S may be a curve in 2D or a spatial surface in 3D, and \mathcal{K} is compact in C when $S \in C^2$. In the next Chapter, we shall discuss various methods for the numerical solution of (1.60) while in Chapters 3 and 4 we shall investigate iterative methods for fast numerical solutions of the resulting boundary element equations. However, when S is only piecewise smooth, an integral equation of the second kind in the form of (1.60) can still be obtained but \mathcal{K} will in general no longer be compact. Results from Chapters 2-4 can not be readily generalized to this case. In Chapters 5 and 6, we shall study specifically the Dirichlet problem defined on a non-smooth domain in the 2D case, where our integral equation is as represented by (1.60) but the operator \mathcal{K} can be split into the sum of a bounded linear operator with norm less than one and a compact operator.

Chapter 2

Numerical solution by boundary element methods

For a general integral equation of the second kind

$$(\mathcal{I} - \mathcal{K})\phi = f \tag{2.1}$$

where $\mathcal{K} : C \rightarrow C$ is a compact linear operator, there are many numerical methods one can use for finding an approximate solution. Refer to [14], [21] and [91]. In this chapter, we first introduce projection type methods such as collocation and Galerkin and then discuss the so-called panel method, which is perhaps the most commonly-used method in engineering applications. The Nyström quadrature method is only briefly discussed. Then we shall introduce the iterated collocation method, which interpolates projection solutions to the continuous space in a similar way to that of the Nyström extension and yields globally a higher order of convergence. Finally in this chapter, we discuss the important problem of numerical integration.

2.1 Projection type methods

The main idea of projection type methods for solving integral equations of the second kind is first to assume that the solution is in some finite dimensional space spanned by a set of basis functions, and then to select a particular linear combination of the basis functions by forcing the approximate solution to have a small residual for the projected integral equation on this space. From the general schema, we obtain the well-known methods of collocation and Galerkin. However in the collocation method, the projection involved is interpolatory whereas for the Galerkin method, it is orthogonal.

Let C_n be a finite dimensional space and \mathcal{P}_n a bounded projection operator from C onto C_n , i.e., \mathcal{P}_n is a bounded linear operator from C to C_n ; with $\mathcal{P}_n x = x$, $\forall x \in C_n$. Then a projection method for solving $(\mathcal{I} - \mathcal{K})\phi = f$ in the space C_n is to find $\phi_n \in C_n$ such that

$$(\mathcal{I} - \mathcal{P}_n \mathcal{K})\phi_n = \mathcal{P}_n f. \quad (2.2)$$

Let the residual of ϕ_n be denoted by¹

$$r_n = f - \phi_n + \mathcal{K}\phi_n. \quad (2.3)$$

Then (2.2) is equivalent to $\mathcal{P}_n r_n = 0$. To provide an error analysis for (2.2), we subtract it from (2.1), giving

$$\phi - \phi_n = (\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1}(\phi - \mathcal{P}_n \phi) \quad (2.4)$$

and

$$\|\phi - \phi_n\| \leq \|(\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1}\| \|\phi - \mathcal{P}_n \phi\|, \quad (2.5)$$

¹We implicitly assume that $\mathcal{K} : L_\infty \rightarrow C$ is compact (see [93]), where L_∞ is the space of essentially bounded functions.

where the supremum norm $\|\cdot\|_\infty$ is used. It can be shown that for the compact operator \mathcal{K}

$$\|(\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1}\| \leq c, \quad n \text{ sufficiently large,} \quad (2.6)$$

provided that a pointwise convergence result holds, that is provided

$$\lim_{n \rightarrow \infty} \|(\varphi - \mathcal{P}_n \varphi)\| = 0, \quad \forall \varphi \in C. \quad (2.7)$$

In (2.6), c is some genetic constant which is dependent on \mathcal{K} only; see [14, Ch.2.2]. Consequently, the sufficient condition (2.7) guarantees the norm convergence of ϕ_n to ϕ , as $n \rightarrow \infty$. We now specify the choice of the projection operator \mathcal{P}_n .

For simplicity, let us consider the 1D case (corresponding to 1D integrals arising from 2D boundary value problems), since the extension to higher dimensions is straightforward. In this case the equation (2.1) may be rewritten as

$$(\mathcal{I} - \mathcal{K})\phi = f, \quad a \leq s \leq b, \quad (2.8)$$

where $\mathcal{K}\phi = \int_a^b K(s, t)\phi(t)dt$.

We shall define a piecewise polynomial space $S^{n,r}$ to specify and replace C_n . For any positive integer n , let

$$\Pi_n : a = \eta_0 < \eta_1 < \cdots < \eta_{n-1} < \eta_n = b \quad (2.9)$$

be a mesh, and for $1 \leq i \leq n$ set $I_i = (\eta_{i-1}, \eta_i]$, $h_{(i)} = \eta_i - \eta_{i-1}$ and $h_n = \max_{1 \leq j \leq n} h_{(j)}$. Assume that $h_n \rightarrow 0$ as $n \rightarrow \infty$. The choice of Π_n in general should depend upon the smoothness of solution ϕ and will be specified later. With r a positive integer, let $S^{n,r}$ denote the space of piecewise polynomials of order r (or degree $\leq r-1$). That is, $u \in S^{n,r}$ if and only if u , on each subinterval I_i , is a polynomial of order r . There are no continuity restrictions imposed on $S^{n,r}$ i.e. discontinuity is permitted at the nodes $\{\eta_j\}_1^{n-1}$.

Let us assume that $S^{n,r}$ has $d-1$ continuous derivatives on $[a, b]$ with $0 \leq d < r$, to determine its dimensionality. Then it can be shown that $N_n = \dim(S^{n,r}) = (n-1)(r-d)+r$. Refer to [63]. Often $d = 0$ is chosen (*i.e.* the case of discontinuous piecewise polynomials²) so we have $N_n = nr$. Now let us denote by $\{\psi_j\}_1^{N_n}$ the basis functions for the space $S^{n,r}$. Obviously any function $u \in S^{n,r}$ may be expressed as

$$u(s) = \sum_1^{N_n} a_j \psi_j(s), \quad a \leq s \leq b. \quad (2.10)$$

In order to use $S^{n,r}$ for practical approximations, we need to specify it further. To this end, let us introduce r distinct points on each subinterval I_i ($i = 1, \dots, n$) as follows :

$$s_{ij}^n = \eta_{i-1} + \xi_j h_{(i)}, \quad 1 \leq j \leq r, \quad (2.11)$$

where $\{\xi_j\}_1^r$ are the nodes of some integration rule on $[0, 1]$ with

$$0 \leq \xi_1 < \xi_2 < \dots < \xi_r \leq 1.$$

Then in the space $S^{n,r}$, any continuous function $v \in C$ may be approximated by v_n , a piecewise Lagrange polynomial interpolating v at nodes $\{s_{ij}^n\}_{j=1}^r$ on each subinterval I_i ($i = 1, \dots, n$). In details, we may write

$$v_n(s) = \sum_{i=1}^n \sum_{j=1}^r \ell_{ij}(s) v(s_{ij}^n), \quad s \in [a, b], \quad (2.12)$$

where

$$v_n(s_{ij}^n) = v(s_{ij}^n) \text{ and } \ell_{ij}(s) = \begin{cases} 0, & s \notin I_i, \\ \prod_{\substack{m=1 \\ m \neq j}}^r \frac{s - s_{im}^n}{s_{ij}^n - s_{im}^n}, & s \in I_i, \end{cases}$$

²In this case, we arbitrarily assume that functions in $S^{n,r}$ are left-continuous at every node except $\eta = \eta_0$ and right-continuous at $\eta = \eta_0$.

for $i = 1, \dots, n$ and $j = 1, \dots, r$. Note that we have $N_n = nr$ when $d = 0$ is chosen (e.g. when $\xi_1 \neq 0$ and $\xi_r \neq 1$). We may now view the space $S^{n,r}$ as spanned by the independent basis functions $\{\psi_j\}_1^{N_n}$ with $\psi_j(s) = \ell_{\nu m}(s)$ for $j = 1, \dots, N_n$, $\nu = \text{INT}[(j-1)/r] + 1$ and $m = j - (\nu - 1)r$. For convenience wherever possible, we shall write $\{s_j^n\}_{j=1}^{N_n}$ or simply $\{s_j\}_1^{N_n}$ for the nodes $\{s_{ij}^n\}_{j=1}^r$ with $i = 1, \dots, n$ (after collection and re-numbering). The specific space $S^{n,r}$, as just defined, will be used throughout the thesis.

The collocation method

To find the approximate solution ϕ_n to the integral equation (2.8) in $S^{n,r}$ by the collocation method, let us define our projection operator $\mathcal{P}_n : C + S^{n,r} \rightarrow S^{n,r}$ by³

$$\mathcal{P}_n u(s) = \sum_1^{N_n} u_j \psi_j(s), \quad a \leq s \leq b. \quad (2.13)$$

with $u_j = u(s_j)$. Applying the operator \mathcal{P}_n to both sides of (2.3), we then collocate at points s_i , $i = 1, 2, \dots, N_n$, giving

$$\sum_{j=1}^{N_n} \phi_j [\psi_j(s_i) - \int_a^b K(s_i, t) \psi_j(t) dt] = f(s_i), \quad (2.14)$$

for $i = 1, 2, \dots, N_n$, with $\psi_j(s_i) = 0$ if $i \neq j$ and $\psi_i(s_i) = 1$.

As mentioned before, the order of convergence of ϕ_n to ϕ will depend on the smoothness of ϕ as well as the mesh Π_n . A simple choice for Π_n is the uniform mesh with $\{\eta_i\}$ defined by

$$\eta_i = a + \frac{i}{n} \cdot (b - a), \quad i = 0, \dots, n. \quad (2.15)$$

³Since $S^{n,r}$ is not a subspace of C , it is natural to require $\mathcal{P}_n : C + S^{n,r} \rightarrow S^{n,r}$. This will be consistent with the other assumption that $\mathcal{K} : L_\infty \rightarrow C$ (or $\mathcal{K} : C + S^{n,r} \rightarrow C$).

Proof. As in the proof of Theorem 2.1, we only need to show that

$$\|\phi - \mathcal{P}_n\phi\| = O(h_n^r).$$

However this now follows from [81] using the graded mesh (2.16) with $q \geq r/\beta$.

Thus (2.17) is proved. \square

For a more complete analysis, we refer to [25] and [89] and the references therein.

In Chapter 5, we shall present the convergence analysis for the collocation method based on similar graded meshes when the non-smoothness of the solution is due to the non-smooth boundaries.

The Galerkin method

To introduce the Galerkin method, we define the inner product of two functions u and v by

$$(u, v) = \int_a^b u(t)v(t)dt, \quad (2.18)$$

and a new projection operator $Q_n : C + S^{n,r} \rightarrow S^{n,r}$ by

$$Q_n u(s) = \sum_{j=1}^{N_n} (u, \psi_j) \psi_j(s), \quad a \leq s \leq b. \quad (2.19)$$

The Galerkin method then requires $Q_n r_n = 0$ (refer to (2.3)), giving rise to a linear system of equations

$$\sum_{j=1}^{N_n} \phi_j \left[\int_a^b \psi_i \psi_j ds - \int_a^b \int_a^b K(s, t) \psi_j(t) \psi_i(s) dt ds \right] = \int_a^b f(s) \psi_i(s) ds, \quad (2.20)$$

for $i = 1, 2, \dots, N_n$. Numerical analysis of the Galerkin method is fairly complete, which may be the reason why it is very widely used by numerical analysts; see [50] and [92] and the references given there. Convergence orders are similar to those of collocation methods. However, Galerkin methods are expensive to implement

and collocation methods are more often used in practice. So we shall not pursue the former any further in the thesis.

The panel method

To conclude the section, we discuss the panel method which is commonly used in engineering applications; (refer to [10] and [23]). This method can be viewed as the discrete collocation method of a low order (*e.g.* with $r = 1$).

Often the method is introduced as follows. Consider a typical boundary integral equation from reformulation of a 3D boundary value problem, as given by (1.60)

$$\phi(p) - \int_S K(p, q)\phi(q)dS_q = f(p), \quad p \in S, \quad (2.21)$$

which is assumed to be solvable on the given boundary $S \subset R^3$. Approximate first of all the boundary S by \tilde{S} , where $\tilde{S} = \cup \tilde{S}_j$ is a piecewise smooth boundary (often \tilde{S}_j 's are flat linear or quadratic panels). In doing so our equation (2.21) changes to

$$\tilde{\phi}(p) - \int_{\tilde{S}} K(p, q)\tilde{\phi}(q)dS_q = f(p), \quad (2.22)$$

or

$$\tilde{\phi}(p) - \sum_j \int_{\tilde{S}_j} K(p, q)\tilde{\phi}(q)dS_q = f(p).$$

Note that because the boundary \tilde{S} is non-smooth, the integral operator defined on it may not be compact and the solution of the boundary integral equation (2.22) may not be smooth; (refer to Chapter 5). Equation (2.22) is then discretized using a low order projection method (often based on piecewise constant collocations) to yield the numerical solution $\tilde{\phi}_n(p)$.

This approach does not allow easy analysis of the numerical results since $\|\phi - \bar{\phi}\|$ is not easy to measure and $\|\bar{\phi} - \bar{\phi}_n\|$ cannot be estimated by classical analysis as the operator on \bar{S} may not be compact. In particular the numerical theory introduced in this chapter is not applicable. The error $\|\phi - \bar{\phi}\|$ in fact determines the choice of numerical methods to be used for numerical solution of (2.22) and hence high order numerical methods may not be needed.

However all these theoretical difficulties can be avoided if the panel method is introduced in a different way. We prefer the following formal introduction of the method. Consider again the equation (2.21). Suppose that we have a partition of S , *i.e.*, a family $\{\Delta_1, \dots, \Delta_n\}$ of disjoint nonempty simply connected subsets of S such that

$$S = \bigcup_1^n \Delta_i. \quad (2.23)$$

Define $S^{n,1}$ to be the space of piecewise constant elements with basis functions

$$\psi_i(p) = \begin{cases} 1, & p \in \Delta_i; \\ 0, & p \notin \Delta_i. \end{cases} \quad (2.24)$$

Then in $S^{n,1}$, the solution function ϕ is approximated by

$$\phi_n(p) = \sum_1^n \gamma_i \psi_i(p), \quad (2.25)$$

where the coefficients γ_i are determined by application of a collocation procedure.

Choose one collocation point p_i in each subregion Δ_i . This yields a linear system of equations for γ_i

$$\gamma_j - \sum_1^n \gamma_i \int_{\Delta_i} K(p_j, q) dS(q) = f(p_j), \quad j = 1, \dots, n. \quad (2.26)$$

Now classical analysis is applicable for error analysis and the remaining problem is in the accurate evaluation of integrals over each surface element Δ_i . Those

integrals, the surface elements of which can be mapped onto some regular domains such as triangles or rectangles, are transformed into simple integrals before numerical integration (§2.3). Other integrals can also be transformed into simple integrals using approximate mappings, which may be found via piecewise spline interpolations. Therefore errors in surface approximations contribute to numerical integration errors. Refer to [10], [15], [88] and §2.3. Note that the discussion here applies also to higher order collocation methods.

Next we shall show how to obtain continuous approximations to solution ϕ .

2.2 Nyström interpolation and iterated projections

In this section we consider the iterated collocation approximation ϕ_n^* , which is closely related to the projection solution ϕ_n . Since ϕ_n^* often converges to the exact solution ϕ faster than ϕ_n , it is particularly useful and attractive. The underlying idea is in fact very similar to the Nyström method, which we shall now briefly introduce. The method will be used in numerical tests of §3.5.1.

The Nyström method

Let us concentrate on the 1D equation (2.8). Denote by $\{\omega_j, t_j\}_1^n$ a quadrature rule⁴, *i.e.*,

$$\int_a^b \vartheta(t) dt = \sum_1^n \omega_j \vartheta(t_j) + \text{Error term}, \quad (2.27)$$

⁴In general, we may use a composite rule based on a chosen quadrature rule. For example, we may first set up a mesh such as Π_n in (2.9) and then apply an r point quadrature rule $\{\omega_j, t_j\}_1^r$ to each subinterval I_i with the total integration nodes $N_n = nr$. The Nyström method defined in this particular way is actually used in later Chapters.

which is assumed to converge for any $\vartheta \in C$ (space of continuous functions). Assume that $t_j \in [a, b]$ for all j . Then such a rule can be used to approximate (2.8) by

$$\phi_n(s) - \sum_{j=1}^n \omega_j K(s, t_j) \phi_n(t_j) = f(s), \quad a \leq s \leq b, \quad (2.28)$$

which needs to be solved for $\phi_n(s)$. To solve (2.28) as a functional equation, we set $s = t_i$ ($i = 1, \dots, n$), giving a system of equations

$$\phi_n(t_i) - \sum_{j=1}^n \omega_j K(t_i, t_j) \phi_n(t_j) = f(t_i), \quad i = 1, \dots, n, \quad (2.29)$$

whose solution vector $[\phi_n(t_1), \dots, \phi_n(t_n)]^T$ gives the solution of (2.28) for all $s \in [a, b]$ by

$$\phi_n(s) \stackrel{\text{def}}{=} \sum_{j=1}^n \omega_j K(s, t_j) \phi_n(t_j) + f(s). \quad (2.30)$$

The method of solving equation (2.8) by seeking an approximate solution ϕ_n from C itself is called the Nyström quadrature method. Furthermore, equation (2.30) is referred to as the *Nyström extension* as it can be used to yield $\phi_n(s)$ once $\phi_n(t_j)$ are known. We refer to [11] and [14] for further analysis of the method. The method is usually considered to be suitable and efficient for integral equations with a well behaved kernel $K(s, t)$. Its modification referred to as the *product integration method* is more robust, of which the iterated projection (collocation) method is a special case. Refer to [31], [89] and [91]. In particular, the collocation method may be viewed as a Nyström method; see [14].

Nyström interpolation

Recall that the collocation approximation $\phi_n = \mathcal{P}_n \phi \in S^{n,r}$ is defined by (2.13) and (2.14). Once ϕ_n is obtained (or $\phi_n(s_j)$ for $j = 1, \dots, N_n$ are obtained), we

may define, referring back to (2.1), a new approximation (the iterated collocation)

$\phi_n^* \in C$ by

$$\phi_n^* \stackrel{\text{def}}{=} f + \mathcal{K}\phi_n. \quad (2.31)$$

The process of (2.31) is called the *Nyström interpolation* (refer to (2.30)). Such an interpolation is essential in developing multigrid methods in Chapter 3, where we use (2.31) (referred to as the Picard iteration) as a way of transferring approximate solutions between grids as well as smoothing out the residuals.

Iterated projections

Assume that \mathcal{K} is compact from L_∞ to C as well as from C to C (although the compactness of \mathcal{K} from $C \div S^{n,r}$ to C is sufficient in the context⁵). It follows immediately from (2.2) and (2.31) that

$$\phi_n = \mathcal{P}_n \phi_n^* \quad (2.32)$$

so that ϕ_n and ϕ_n^* coincide at collocation points $\{s_j\}_1^{N_n}$. It follows in turn that ϕ_n^* satisfies an equation of the second kind

$$(\mathcal{I} - \mathcal{K}\mathcal{P}_n)\phi_n^* = f, \quad (2.33)$$

where the compactness of $\mathcal{K}\mathcal{P}_n : C \rightarrow C$ follows from our assumption. We now state an important result concerning the convergence analysis of the iterated collocation approximations.

THEOREM 2.3

Assume that $f \in C$, $\{\xi_j\}_1^r$ (used in defining the projection operator \mathcal{P}_n of (2.32))

⁵Note that $S^{n,r} \subset L_\infty$.

are chosen to be the $[-1, 1]$ Gauss-Legendre quadrature points shifted to $[0, 1]$ and

$$\lim_{s \rightarrow \tau} \int_a^b |K(s, t) - K(\tau, t)| dt = 0.$$

Then if $\phi \in C^l$ ($0 < l \leq 2r$) and $K_s(t) = K(s, t) \in C^m$ ($0 < m \leq r$) with

$$\max_{t \in [a, b]} \left| \frac{\partial^m K_s(t)}{\partial t^m} \right| \leq c, \quad c : \text{generic constant},$$

then

$$\|\phi - \phi_n^*\| = O(h_n^\gamma), \quad \text{with } \gamma = \min(l, r + m).$$

Proof. The proof follows immediately from [50]. □

Note from Theorem 2.3 that the iterated collocation solution may exhibit up to $O(h_n^{2r})$ convergence, which is usually referred to as the superconvergence (because $O(h_n^{2r})$ is the best possible order achievable using the space $S^{n,r}$). If the solution ϕ is not very smooth⁶, non-uniform meshes such as the graded meshes defined by (2.16) may have to be adopted to obtain superconvergence results. One simple application of the superconvergence analysis is that the collocation solution ϕ_n may exhibit higher order of convergence at collocation points $\{s_j\}_1^{N_n}$ due to (2.32). We refer to [25], [31] and [89] and the references there for more details.

2.3 Numerical integration

In general to implement boundary integral equation methods, all integrals involved have to be numerically evaluated, because usually it is either impossible or inefficient to try to find the analytical forms of integrals. The work of evaluating these integrals, or setting up the discrete boundary integral equations, and

⁶For the particular integral equation of (2.8), a weakly singular kernel $K(s, t)$ determines the possible presence of non-smooth solutions ϕ ; see [48].

that of the subsequent solution of linear system of equations are the two most expensive parts of a boundary integral equation method. For the latter problem, the solution of linear systems, iterative methods have been developed for fast and efficient solutions. Refer to Chapters 3, 4 and 6.

The problem of numerical integration is an important and well documented subject. Many fundamental methods may be found in [39]. As for numerical integrations in implementation of boundary element methods, very extensive discussion has been recently given in [17] and [78]. In this section however, we do not attempt to present a comprehensive survey. Material to be presented will only be sufficient in carrying out numerical experiments in later chapters. We refer to [17], [23, §3], [39] and [78] and the references therein for a wider exposition.

1) Introduction

To assist the practitioner with the choice of suitable integration rules, let us classify the different cases. Write a typical integral defined on some panel of S as

$$I(p) = \int_{\Delta} K(p, q)w(q)dS_q, \quad p \in S, \quad (2.34)$$

where $K(p, q)$ is usually a function of distance $r = |p - q|$ and $w(q)$ represents a smooth function (depending on the numerical method used for discretization).

Then to evaluate $I(p)$, $p \in S$, we have to consider the following cases :

- (a) $K(p, q)$ is well-behaved, (when p is away from Δ);
- (b) $K(p, q)$ is nearly singular, (when p is close to but not in Δ);
- (c) $K(p, q)$ is singular at p , (when p is in Δ).

For the case (a), the Gauss-Legendre rule is usually applied. However other more efficient methods are also available; (see [39]). For the case (b), the com-

posite Gauss-Legendre rule (or an appropriate adaptive rule) may be applied to overcome the near singularity. Other methods may also be considered; (refer to [17]). In the case (c), there are three possible situations to be dealt with. (i) If $I(p)$ has a Cauchy singularity at $q = p$, it is often a good idea if possible to carry out some analysis of the integral before using numerical quadrature rules; (refer to [23, §3] and the references therein). (ii) If the singularity is apparent, or removable using the singularity subtraction technique, the case will be more amenable to numerical approximations. (iii) Otherwise the ERF rule may always be considered for the evaluation of integrals with a weakly singular integrand. For this case (iii), there are other useful techniques one may consider, such as the singularity cancelling transformation for 1D integrals and the polar coordinate transformation for 2D integrals. We refer to [23, §3] and the references there for further discussions.

Next we shall first discuss the problem of transformation of boundary integrals into ordinary integrals. Then we discuss the Gauss-Legendre rule and the singularity subtraction technique. Finally we describe the ERF rule for integrands with end point singularities.

2) Boundary integrals

Integrals arising from practice are often defined on some small panel (element) of boundary S , as discussed in 1). To integrate either analytically or numerically such integrals, it is necessary to reduce them to some regular forms, i.e., transform them to simple integrals on triangles or rectangles; (refer to the discussion on the panel method in §2.1). The ideal situation is when a parametric representation exists which maps bijectively the boundary element onto a segment of line

(1D) or a rectangle of plane (2D). But when such a mapping is not easily available, the curve-fitting methods such as interpolations with splines will have to be incorporated to provide an approximate mapping. See [10], [15], [23, §3], [27] and [28] for more details. Below we assume that such a parametric representation (mapping) exists and go on to present some details from vector analysis.

1D case. Suppose that we have a transformation

$$\left. \begin{aligned} x &= x(t) \\ y &= y(t) \end{aligned} \right\}, \quad t \in [a, b]$$

which maps bijectively $[a, b]$ onto the i th curve segment Δ_i (with partition $S = \bigcup_1^n \Delta_i$). Define functions

$$d_1(t) = \frac{d}{dt}y(t), \quad d_2(t) = -\frac{d}{dt}x(t), \quad \text{and } g(t) = \sqrt{d_1^2 + d_2^2},$$

for $t \in [a, b]$. Then the element of length becomes

$$dS = g(t)dt,$$

and the outward normal at point $q = (x, y)$ takes the form

$$n_q = (d_1, d_2)/g(t).$$

Therefore on Δ_i , the two layer potentials are respectively transformed to

$$\begin{aligned} (L_k \sigma)_i(p) &= \int_a^b \sigma(q) G_k g(t) dt, \quad p = (x_0, y_0), \\ (M_k \sigma)_i(p) &= \int_a^b \sigma(q) \frac{\partial G_k}{\partial r} \left(\frac{\partial r}{\partial x} d_1 + \frac{\partial r}{\partial y} d_2 \right) dt, \quad p = (x_0, y_0), \end{aligned}$$

where $q = (x, y)$, $G_k = G_k(p, q) = \frac{i}{4} H_0^{(1)}(kr)$ and $r = \sqrt{(x - x_0)^2 + (y - y_0)^2}$.

2D case. Suppose that we have for S a partition $S = \bigcup_1^n \Delta_i$, as in (2.23),

and assume that the parametric representation

$$\left. \begin{aligned} x &= x(\xi, \eta) \\ y &= y(\xi, \eta) \\ z &= z(\xi, \eta) \end{aligned} \right\}, \quad (\xi, \eta) \in R_i$$

defines an invertible mapping from a rectangle R_i in ξ - η plane to the surface element Δ_i . Define also functional determinants

$$D_1 = \begin{vmatrix} \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \end{vmatrix}, \quad D_2 = \begin{vmatrix} \frac{\partial z}{\partial \xi} & \frac{\partial x}{\partial \xi} \\ \frac{\partial z}{\partial \eta} & \frac{\partial x}{\partial \eta} \end{vmatrix}, \quad D_3 = \begin{vmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{vmatrix},$$

which are assumed not to vanish simultaneously, and the Jacobian function

$$J(\xi, \eta) = \sqrt{D_1^2 + D_2^2 + D_3^2}.$$

Then the element of area becomes

$$dS = J(\xi, \eta) d\xi d\eta$$

and the outward normal at $q = (x, y, z)$ becomes

$$n_q = -(D_1, D_2, D_3)/J(\xi, \eta).$$

Similar to the 1D case, on each Δ_i , the two layer potentials become respectively

$$(L_k \sigma)_i(p) = \iint_{R_i} \sigma(q) G_k J(\xi, \eta) d\xi d\eta, \quad p = (x_0, y_0, z_0),$$

$$(M_k \sigma)_i(p) = \iint_{R_i} \sigma(q) \frac{\partial G_k}{\partial r} \left(\frac{\partial r}{\partial x} D_1 + \frac{\partial r}{\partial y} D_2 + \frac{\partial r}{\partial z} D_3 \right) d\xi d\eta, \quad p = (x_0, y_0, z_0),$$

where $q = (x, y, z)$, $G_k = G_k(p, q) = \frac{e^{ikr}}{4\pi r}$ and $r = \sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2}$.

3) Gauss-Legendre rule

The Gauss-Legendre rule is perhaps the most commonly-used numerical quadrature rule in boundary integral equation methods (or BEM's). It requires the integrand to be very smooth to yield high orders of accuracy. Since the 1D integration rule can often be naturally extended to 2D integration, we shall concentrate on the 1D case only, writing a typical 1D integral as

$$I = \int_{-1}^1 f(x)dx. \quad (2.35)$$

For an integrand defined on $[a, b]$, a change of coordinates by

$$x = \frac{b-a}{2}y + \frac{b+a}{2}$$

will map $[a, b]$ bijectively to $[-1, 1]$, *i.e.*,

$$\int_a^b f(x)dx = \frac{b-a}{2} \int_{-1}^1 f\left(\frac{b-a}{2}y + \frac{b+a}{2}\right)dy.$$

The classical Gauss-Legendre integration formula for (2.35) is given by

$$I = \sum_1^n w_j f(x_j) + E_n(f),$$

where abscissae $\{x_j\}_1^n$ in $[-1, 1]$ are the n real and simple zeros of the orthonormal Legendre polynomials P_n^* and weights $\{w_j\}_1^n$ are determined by

$$w_j = -\frac{c_{n+1}}{c_n} \frac{1}{P_{n+1}^*(x_j)P_n^{*\prime}(x_j)}$$

with the error term

$$E_n(f) = \frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi), \quad -1 < \xi < 1,$$

for $f \in C^{2n}[-1, 1]$ and c_n is the leading coefficient of $P_n^*(x) = c_n x^n + \dots$. The orthogonal Legendre polynomials $P_n(x)$ are known to satisfy the three term recurrence

$$P_{n+1}(x) = \frac{n}{n+1} [x P_n(x) - P_{n-1}(x)] + x P_n(x)$$

and their derivatives satisfy

$$(1 - x^2)P'_{n+1}(x) = n[P_{n-1}(x) - xP_n(x)],$$

with $P_0(x) \equiv 0$ and $P_1(x) = x$. The orthonormal Legendre polynomials are defined by $P_n^*(x) = \frac{2n+1}{2}P_n(x)$. The zeros of $P_n(x)$ may be calculated by the Newton-Raphson iteration, i.e., for x_j

$$x_j^{(l+1)} = x_j^{(l)} - \frac{P_n(x_j^{(l)})}{P'_n(x_j^{(l)})}, \quad l = 0, 1, \dots$$

with initial guess $x_j^{(0)} = (1 - \frac{1}{8}n^{-2} + \frac{1}{8}n^{-3})\cos(\frac{4j-1}{4n+2})$ because $x_j = x_j^{(0)} + O(n^{-4})$.

For a listing of a FORTRAN routine to generate $\{x_j\}_1^n$ and $\{w_j\}_1^n$, refer to [39, p.487]. The abscissae $\{x_j\}$ are located symmetrically in $[-1, 1]$ and weights $\{w_j\}$ corresponding to symmetric points are equal. Note that $n = 1$ gives the familiar mid-point rule, whose composite form is often used.

4) Singularity subtraction

One important technique in treating the singular integrals before numerical integration is the *singularity subtraction*, which is also useful in solving integral equations(see [19]). Suppose that an integrand $g(x)$ is integrable, its integral can be found accurately or analytically and function $f(x) - g(x)$ is not singular. Then the general method is to subtract from the singular integrand $f(x)$ the function $g(x)$ to rewrite

$$\int f(x)dx = \int g(x)dx + \int (f(x) - g(x))dx.$$

The second integral on the right hand side of the above equation is now more amenable to numerical approximations. The choice of $g(x)$ determines the smoothness of the function $f(x) - g(x)$. One simple application is given as follows

$$\int_0^1 H_0^{(1)}(x)dx = \int_0^1 g(x)dx + \int_0^1 (H_0^{(1)}(x) - g(x))dx$$

with the first integrand $g(x) = \frac{2i}{\pi} \log(\frac{x}{2})$ integrable and the second $H_0^{(1)}(x) - g(x)$ non-singular. The function $H_0^{(1)}(x) - g(x)$ belongs to C^1 . However if we choose $g(x) = \frac{2i}{\pi} [1 - \frac{x^2}{4}] \log(\frac{x}{2})$, then the function $H_0^{(1)}(x) - g(x)$ will belong to C^3 . In general, $g(x)$ is chosen from certain series expansions of function $f(x)$. Refer to [23, §3], [39] and [78] for more details.

5) ERF integration rule

The Gauss-Legendre rule may be applied to (2.35) with integrands having no singularities in $(-1, 1)$ as well as those with smooth integrands, while the simpler ERF rule, as studied in [2], is quite useful for integrands with end point singularities (at $x = -1$ or 1). Consider (2.35) where $f(x)$ may possess singularities at either or both end points ± 1 . The ERF rule is based on a variable transformation

$$x = \operatorname{erf}(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-u^2} du$$

to change (2.35) into

$$I = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(\operatorname{erf}(t)) e^{-t^2} dt.$$

Notice that the new integrand is now non-singular since it is dominated by e^{-t^2} for large $|t|$ near possible singularities (shifted to $\pm\infty$). Consequently, the integral may be approximated very accurately by a composite trapezium rule to yield the $2m+1$ point ERF rule :

$$I \approx \sum_{-m}^m w_j f(x_j)$$

with $w_j = \frac{2h}{\sqrt{\pi}} e^{-(jh)^2}$ and $x_j = \operatorname{erf}(jh)$. Usually $\operatorname{erf}(x)$ may be numerically computed (*e.g.* by NAG routine S15AEF) and the choice of the step size h and the number m depends on the strength of the singularity and the required accuracy. See [2] for the theoretical choice and further details.

Chapter 3

Multigrid Methods for Smooth Integral Equations

In Chapter 2, we have presented numerical methods for solving integral equations of the second kind, concentrating mainly on the iterated projection method and the Nyström method. Both methods, when applied to linear integral equations such as (1.60), will produce an intermediate linear system of equations (usually with full and complex matrix). The solution of the linear system is then used through the Nyström type interpolation to yield the final approximate solution. When the order N of the linear system becomes large, direct methods such as Gaussian elimination with partial pivoting, requiring $O(N^3)$ operations, will be too expensive to use. In this chapter, we introduce and investigate a class of efficient multigrid type methods to solve integral equations iteratively, reducing the computational cost to $O(N^2)$. Modified variants will also be suggested based on the existing methods and numerical experiments will be carried out to show their efficiency.

3.1 Introduction

Multigrid methods for a functional equation are iterative schemes that work with a sequence of computational grids of increasing refinement. The solutions of the different but related problems on these grids interact with each other to obtain iterative approximations to the continuous solution of the functional equation. In particular, two grid methods are the simplest examples of multigrid hierarchy. All these methods follow the residual correction principle (RCP, §3.2), combined with fine grid relaxations for smoothing and coarse grid corrections for improvement. Such multigrid ideas have been studied and applied to the solution of partial differential equations (PDE's); see [1], [34] and [96], and the solution of the integral equations; see [13], [52], [58] and [71]. However, as mentioned earlier, discretization of integral equations usually generates non-sparse systems of equations, being different from that of PDE's, which produces sparse coefficient matrices. Here we present a systematic analysis of multigrid methods, as applied to integral equations.

To introduce a functional equation and allow at the same time wider generality (*e.g.* in dimensionality), we define our integral equation in operator notation as

$$(\mathcal{I} - \mathcal{K})u = f(p), \quad p \in S, \tag{3.1}$$

where $\mathcal{K} : X \rightarrow X$ is a bounded linear integral operator over the Banach space X and is given explicitly by

$$(\mathcal{K}\varphi)(p) = \int_S K(p, q)\varphi(q)dS_q, \quad p \in S,$$

with S being a contour in 2D or a closed surface in 3D (refer to (1.60) and (2.8)).

Here we choose the numerical technique to be either the iterated collocation method or the Nyström method. In any case, let us denote by $\{G[\ell]\}_{\ell=1}^{\infty}$ a sequence of grids (with number of grid points $\{N_\ell\}_{\ell=1}^{\infty}$ such that $N_1 < N_2 < \dots$), on each of which the approximate solution of (3.1) is denoted by u_ℓ and the approximate operator by \mathcal{K}_ℓ . This implies that $G[\ell]$ either represents the collection of all N_ℓ collocation points with $\mathcal{K}_\ell = \mathcal{K}\mathcal{P}_\ell$ (for some projection operator \mathcal{P}_ℓ) for the iterated collocation method; or represents the union of all integration nodes with the Nyström method. Refer to §2.2. Symbolically we write the approximate equation as

$$(\mathcal{I} - \mathcal{K}_\ell)u_\ell = f, \quad f \in X, \quad \ell = 1, 2, \dots, \quad (3.2)$$

where the subscript ℓ has been used to indicate that a quantity is defined on grid $G[\ell]$; a notation which will be used from here on whenever no confusion may arise. For each ℓ , the above equation describes the process of discretization, the solution of the discrete problem at $G[\ell]$ points (*i.e.* the solution of a square linear system), and the subsequent Nyström interpolation (§2.4.2). We shall refer to such a process as the $G[\ell]$ problem. To solve a $G[m]$ problem by multigrid methods ($m > 1$), we make full use of available information from solving $G[m-1]$, $G[m-2]$, \dots , $G[1]$ problems.

In §3.2, we introduce the residual correction principle (RCP), which provides a suitable framework for the motivation and convergence analysis of two grid methods (§3.3) and multigrid methods (§3.4). Modified variants naturally follow the standard methods. Numerical tests are carried out in §3.5 for both a simple model problem and a 2D exterior Dirichlet problem for the Helmholtz equation. In §3.6, we discuss the very important problem of achieving the full efficiency of

iterative methods.

3.2 Residual correction principle

Consider the problem of solving a functional equation

$$\mathcal{A}u = f \tag{3.3}$$

where $\mathcal{A} : X \rightarrow X$ is any non-singular linear operator over the Banach space X .

In particular, X may be the space C^n and \mathcal{A} may be thought of as $(\mathcal{I} - \mathcal{K})$ from integral equation (3.1). Now if a related equation

$$\tilde{\mathcal{A}}v = r,$$

with $\tilde{\mathcal{A}} : X \rightarrow X$, can be solved efficiently for arbitrary right hand side $r \in X$, we may attempt to solve (3.3) using the residual correction iterative scheme

$$\begin{aligned} \tilde{\mathcal{A}}u^{(l+1)} &= (\tilde{\mathcal{A}} - \mathcal{A})u^{(l)} + f \\ &= \tilde{\mathcal{A}}u^{(l)} + r^{(l)}, \quad l = 0, 1, 2, \dots, \end{aligned}$$

i.e.

$$\begin{aligned} u^{(l+1)} &= (\mathcal{I} - B\mathcal{A})u^{(l)} + Bf \\ &= u^{(l)} + Br^{(l)}, \quad l = 0, 1, 2, \dots, \end{aligned} \tag{3.4}$$

where $r^{(l)} = f - \mathcal{A}u^{(l)}$ is the *residual* corresponding to the present iterate $u^{(l)}$ and $B = (\tilde{\mathcal{A}})^{-1}$. By induction, it can be shown that

$$u - u^{(l)} = (\mathcal{I} - B\mathcal{A})^l(u - u^{(0)}), \quad l \geq 0.$$

Therefore the sufficient and necessary condition for $u^{(l)}$ to converge to u , starting from an arbitrary initial guess $u^{(0)}$, is that

$$(\mathcal{I} - BA)^l \rightarrow 0, \text{ as } l \rightarrow \infty. \quad (3.5)$$

Clearly $u^{(l)}$ converges to $u = A^{-1}f$ as $l \rightarrow \infty$ if (sufficient condition)

$$\|\mathcal{I} - BA\| < 1, \quad (3.6)$$

or

$$\|(\mathcal{I} - BA)^2\| < 1. \quad (3.7)$$

In linear algebra, when X is chosen to be the finite dimensional Euclidean vector space R^n , the approximate LU factors of the matrix A or any other convenient approximation of A are used as \tilde{A} in order to obtain results correct to within the machine accuracy. See [16, §8.5] for more details.

Denoting $A = \mathcal{I} - \mathcal{K}$ for equation (3.3), we assume that there exists an approximation $\tilde{A} = \mathcal{I} - \tilde{\mathcal{K}}$ to it. Then the application of the residual correction principle yields the following iteration

$$u^{(l+1)} = u^{(l)} + (\mathcal{I} - \tilde{\mathcal{K}})^{-1} r^{(l)}, \quad l = 0, 1, 2, \dots, \quad (3.8)$$

with $r^{(l)} = f - (\mathcal{I} - \mathcal{K})u^{(l)}$. Choosing the approximate operator \tilde{A} or $\tilde{\mathcal{K}}$ differently, by relating them to coarser grids, leads to various multigrid variants, as we shall discuss shortly.

3.3 Two grid methods and their modifications

An early application of the two grid methods for integral equations is due to Hashimoto [55]. There, to solve the equation (3.1) as a $G[m]$ problem with a large

value N_m (say $N_m = r \cdot N$), the inverse of $(\mathcal{I} - \mathcal{K}_n)$ from the $G[n]$ problem with a small value N_n (say $N_n = N$) is used in order to form cheaply an approximate inverse for $(\mathcal{I} - \mathcal{K}_m)$ which is then used in the residual correction scheme (3.4).

Here we shall concentrate on two grid iterative techniques of Atkinson [13] and [14] which lend themselves more readily for generalization to multigrid methods (see §3.4).

(i) Atkinson's two-grid method 1 (TG-1). Consider two discretizations of equation (3.1) in the form (3.2) *i.e.*

$$(\mathcal{I} - \mathcal{K}_l)u_l = f(p), \quad f \in X, \quad (3.9)$$

for $l = m$ and n with $N_m > N_n \geq N_1$ (implying $m > n$). Then Atkinson's method 1 for solving (3.9) with $N_l = N_m$ is based on choosing $\tilde{\mathcal{A}} = (\mathcal{I} - \mathcal{K}_n)$ in (3.8), giving rise to the iterative scheme

$$\begin{aligned} (\mathcal{I} - \mathcal{K}_n)u_m^{(l+1)} &= (\mathcal{K}_m - \mathcal{K}_n)u_m^{(l)} + f \\ &= (\mathcal{I} - \mathcal{K}_n)u_m^{(l)} + r_m^{(l)}, \quad l = 0, 1, 2, \dots \end{aligned} \quad (3.10)$$

For implementation details of (3.10), refer to [14, p.141] and part (iii) in this section. It follows from (3.6) that the convergence of (3.10) is guaranteed if

$$\beta_{n,m}^l = \|(\mathcal{I} - \mathcal{K}_n)^{-1}(\mathcal{K}_m - \mathcal{K}_n)\| < 1. \quad (3.11)$$

But (3.11) cannot in general be proved directly since the convergence of \mathcal{K}_l to \mathcal{K} is usually only pointwise and not uniform (refer to Theorem 1.4). However we see that the convergence of (3.10) is still guaranteed if (a weaker but sufficient condition from (3.7))

$$\rho_{n,m}^l = \|[(\mathcal{I} - \mathcal{K}_n)^{-1}(\mathcal{K}_m - \mathcal{K}_n)]^2\| < 1 \quad (3.12)$$

holds. In fact, the following can be proved using Theorem 1.4 (for compact operators); (see [13] and [14] for the proof)

$$\rho_{n,m}^I \rightarrow 0 \text{ as } N_n, N_m \rightarrow \infty.$$

Therefore the method TG-1 converges when N_n is sufficiently large.

(ii) **Atkinson's two-grid method 2 (TG-2)**. This method is similar to method 1 except that in place of $u_m^{(l)}$ in (3.10) we use $\bar{u}_m^{(l)}$ obtained by one Picard iteration as follows

$$\bar{u}_m^{(l)} = \mathcal{K}_m u_m^{(l)} + f(p), \quad p \in S. \quad (3.13)$$

It can be shown ([90]) that for $\bar{u}_m^{(l)}$ the new residual $\bar{r}_m^{(l)} = \mathcal{K}_m r_m^{(l)}$ which is in general smoother than $r_m^{(l)}$. Atkinson's method 2 (TG-2) can be written as

$$\begin{aligned} (\mathcal{I} - \mathcal{K}_n)u_m^{(l+1)} &= (\mathcal{K}_m - \mathcal{K}_n)f + (\mathcal{K}_m - \mathcal{K}_n)\mathcal{K}_m u_m^{(l)} + f \\ &= (\mathcal{I} - \mathcal{K}_n)u_m^{(l)} + (\mathcal{I} - \mathcal{K}_n + \mathcal{K}_m)r_m^{(l)}, \quad l = 0, 1, 2, \dots \end{aligned} \quad (3.14)$$

Again it follows from (3.6) that the convergence of (3.14) is guaranteed if the iteration operator for (3.14) satisfies

$$\beta_{n,m}^{II} = \|(\mathcal{I} - \mathcal{K}_n)^{-1}(\mathcal{K}_m - \mathcal{K}_n)\mathcal{K}_m\| < 1. \quad (3.15)$$

It is easy to show that (3.15) is true for sufficiently large N_n . Actually the following stronger result can be proved using Theorem 1.4; (see [13] and [14] for the proof)

$$\beta_{n,m}^{II} \rightarrow 0 \text{ as } N_n, N_m \rightarrow \infty.$$

In general TG-2 should have better convergence properties than TG-1, however requiring more operations (roughly twice) per step of iteration.

(iii) **Modified two-grid method (TG-3)**. Here we propose a modified method which is a combination of TG-1 and TG-2. Because of the inherent smoothing properties of compact operators, the Nyström interpolation from $G[n]$ to $G[m]$ via

$$v_m = f + \mathcal{K}_n v_n$$

often renders the expensive residual smoothing in TG-2 unnecessary after the initial few iterations. It follows from (3.13) that $\bar{u}_m^{(l)} = u_m^{(l)} + r_m^{(l)}$ and hence in TG-3 we propose to start as in TG-2 until $\|r_m^{(l)}\|$ is sufficiently small and then revert to the cheaper TG-1 iterations. The convergence of TG-3 is guaranteed by those of TG-2 and TG-1.

The normal implementation of the method TG-3 for general N_n, N_m would require the setting up of four matrices. In practice, we usually choose points of $G[n]$ to coincide with those of $G[m]$, so that we require fewer quantities. For iterated collocation with piecewise constants or the Nyström method in special cases, this is the case if we simply choose $N_m = rN_n$ for some integer ratio r . With such choices of N_m, N_n , we only require the following quantities :

K_m : $N_m \times N_m$ matrix from operator \mathcal{K}_m evaluated at $G[m]$ points;

K_{mn} : $N_m \times N_n$ matrix from operator \mathcal{K}_n evaluated at $G[m]$ points;

K_n : $N_n \times N_n$ matrix from operator \mathcal{K}_n evaluated at $G[n]$ points,

and the vector f_m with $(f_m)_j = f(p_j)$, $p_j \in G[m]$. Then starting from an initial guess $u_m = 0$, we can describe the two grid algorithm for TG-3 as follows :

0) Set $r_m = f_m$, $u_m = 0$, $IR = 0$ and input TOL (tolerance) and EPS (control) and go to step 4);

1) Find the residual on $G[m]$: $r_m = f_m - u_m + K_m u_m$;

- 2) If $IR = 1$ then goto 5);
- 3) If $\|r_m\| \leq EPS$, then $IR = 1$ and goto 5);
- 4) Perform smoothing on $G[m]$: $u_m = u_m \div r_m$ and $r_m = K_m r_m$;
- 5) Restrict the residual r_m to $G[n]$: $r_n = R_m^n r_m$;
- 6) Solve exactly on $G[n]$: $(I - K_n)v_n = r_n$;
- 7) Interpolate v_n to obtain v_m on $G[m]$; $v_m = (r_m \div K_{mn}v_n)$;
- 8) Add on the correction v_m to u_m , $u_m = u_m + v_m$;
- 9) If $\|v_m\| \leq TOL$ exit with solution in u_m ; otherwise go to step 1).

Here the restriction operator R_m^n may be taken to be the so-called injection operator for the iterated collocation method with piecewise constant approximations or the Nyström method in special cases, provided that the points of $G[n]$ are a subset of $G[m]$. But for iterated collocation method with piecewise polynomials of order higher than 1, step 5 may have to be calculated by $r_n = f_n - u_n + K_{nm}u_m$ where K_{nm} is the $N_n \times N_m$ matrix from operator \mathcal{K}_m evaluated at $G[n]$ points and u_n is the solution vector on $G[n]$. In practice, this step may be replaced by a linear interpolation of some appropriate order; refer to [58]. Note that step 6 is in general carried out using a direct solver where the LU decomposition of the matrix is kept for use in each iteration.

Since equation (3.9) with $\ell = n$ is solved by a direct solver (step 6 in the algorithm), the computational cost is $O(N_n^3)$ arithmetic operations. Clearly to maintain the total computing cost at $O(N_m^2)$ level, we should use the criterion that $N_n \leq cN_m^{2/3}$ where c is some small constant. For a fixed value of N_m , increasing N_n

results in increase of the cost of LU factorization but should reduce $\rho_{n,m}^I$ and $\beta_{n,m}^{II}$ hence resulting in faster convergence. On the other hand, taking smaller values for N_n reduces the factorization cost, though increasing the required number of iterations and can also result in the divergence of (3.10) and (3.14). The choice of the optimal ratio N_m/N_n , in order to minimise the solution time, is a problem dependent parameter and somewhat difficult to analyse but will be examined experimentally in §3.5. In the next section on multigrid methods, we will work with a family of grids with decreasing mesh sizes, as set up for (3.2), hence to a large extent alleviating the above problem.

Finally we remark that, although the convergence indicators $\rho_{n,m}^I$ and $\beta_{n,m}^{II}$ can be shown to go to zero as $N_n, N_m \rightarrow \infty$, we may in fact give sharper and more precise bounds for them in terms of step size h_m if we assume that the kernel K of the compact operator is Hölder-continuous of some order; (refer to [72]). Below we shall state one such result.

THEOREM 3.1

Suppose that our 1D integral equation of the second kind is given by

$$u(s) - (\mathcal{K}u)(s) = f(s), \quad 0 \leq s \leq 1, \quad (3.16)$$

where the operator \mathcal{K} defined by $(\mathcal{K}v)(s) = \int_0^1 K(s,t)v(t)dt$ is assumed compact in $C[0, 1]$. Assume that the kernel function satisfies

$$K_s(t) \equiv K(s, t) \in C^{[\alpha], \alpha - [\alpha]} \quad \text{and} \quad K_t(s) \equiv K(s, t) \in C^{[\alpha], \alpha - [\alpha]}$$

for some real number $\alpha \geq 0$, where $[\alpha] = INT(\alpha)$ is the integer part of α . Let us discretize (3.16) by the Nyström method based on the trapezium rule. Then using

two grid methods, there exists an integer $N_0 > 0$ such that for $N_m, N_n \geq N_0$

$$\rho_{n,m}^I = \|[(I - \mathcal{K}_n)^{-1}(\mathcal{K}_m - \mathcal{K}_n)]^2\| \leq cN_m^{-\gamma},$$

$$\beta_{n,m}^{II} = \|(I - \mathcal{K}_n)^{-1}(\mathcal{K}_m - \mathcal{K}_n)\mathcal{K}_m\| \leq cN_m^{-\gamma}$$

where c is a constant independent of N_m and N_n , and $\gamma = \min(2, \alpha)$.

Proof. See [80] for the details. □

3.4 Multigrid variants and their modifications

Here we consider iterative methods which use more than two grids in order to solve (3.2) to the level of the discretization error at the finest grid. For equation (3.2), let us denote, for any integer ℓ (or N_ℓ), an approximate inverse of $\mathcal{A}_\ell \equiv (I - \mathcal{K}_\ell)$ by B_ℓ . Starting with $u_\ell^{(0)}$, the residual correction principle can be used to yield the iterative scheme

$$u_\ell^{(l+1)} = (I - B_\ell \mathcal{A}_\ell)u_\ell^{(l)} + B_\ell f, \quad l = 0, 1, 2, \dots; \quad \ell = 1, 2, \dots \quad (3.17)$$

which converges to the solution of (3.1) provided $\|I - B_\ell \mathcal{A}_\ell\| < 1$. In this notation, the two grid methods TG-1 and TG-2 for the adjacent grids $G[\ell]$, $G[\ell-1]$ use the following approximate inverses respectively :

$$\text{TG-1} \quad B_\ell^{(1)} = (I - \mathcal{K}_{\ell-1})^{-1}, \quad (3.18)$$

$$\text{TG-2} \quad B_\ell^{(2)} = (I - \mathcal{K}_{\ell-1})^{-1}(I - \mathcal{K}_{\ell-1} + \mathcal{K}_\ell) = I + (I - \mathcal{K}_{\ell-1})^{-1}\mathcal{K}_\ell. \quad (3.19)$$

For two grid methods, all coarse grid equations for residual correction are usually solved using direct elimination methods. However each of such functional equations may also be solved by other two grid methods instead of direct methods. Repeating the process, we shall get a nested recursion of two grid methods involving multiple grids. This leads us to multigrid methods.

To be more precise, let us define by $TG(u, v, \gamma_u)$ a γ_u step two grid method operating on two distinct grids $G[u]$ and $G[v]$ (with $u > v$), where $\gamma_u \geq 1$. Here in our two grid method (either TG-1 or TG-2) coarse grid equations on $G[v]$ may be solved by *any method*. We further specify such a method to be *either* the $TG(v, w, \gamma_v)$ method — another two grid method (interacting between $G[v]$ and $G[w]$ with $v > w$) of a fixed step γ_v if $G[v]$ is not yet the coarsest grid; *or* a direct solver if $G[v]$ is already the coarsest grid. Therefore when solving the $G[\ell]$ problem by a $TG(\ell, \ell - 1, \gamma_\ell)$ method, we actually implement a sequence of fixed step two grid methods *i.e.*

$$\begin{aligned} &TG(\ell, \quad \ell - 1, \quad \gamma_\ell), \\ &TG(\ell - 1, \quad \ell - 2, \quad \gamma_{\ell-1}), \\ &\quad \vdots \\ &TG(2, \quad 1, \quad \gamma_2). \end{aligned}$$

On the coarsest grid $G[1]$, we employ a direct solver. Methods so generated are called the multigrid methods. The numbers γ_i , $i = 2, \dots, \ell - 1$ are usually (but not necessarily) chosen to be the same *i.e.* $\gamma_i \equiv \gamma \geq 1$. Such a number γ is the integer indicating the cyclic pattern of a multigrid procedure; see [34] and [52]. If $\gamma = 1$ we have the familiar V-cycling and $\gamma = 2$ is the preferred W-cycling; refer to [52], [96] for further details¹. If the sequence of above two grid methods are of mixed type (either TG-1 or TG-2), we obtain different multigrid variants. Very often these two grids are chosen of the same type. From types TG-1 and TG-2, we obtain the corresponding multigrid methods MG-1 and MG-2 respectively.

All other multigrid variants may be considered to be combinations of MG-1 and

¹The necessity of such a parameter γ can also be seen in the convergence analysis of this section.

MG-2. We shall discuss MG-3 shortly, which is one such combination.

In operator notation, the approximate inverses for MG-1 and MG-2 can be written via

$$\text{MG-1} \quad \begin{cases} B_1^{(3)} = (\mathcal{I} - \mathcal{K}_1)^{-1} \\ B_\ell^{(3)} = Q_{\ell-1}^{(3)}, \quad \ell = 2, 3, \dots \end{cases} \quad (3.20)$$

$$\text{MG-2} \quad \begin{cases} B_1^{(4)} = (\mathcal{I} - \mathcal{K}_1)^{-1} \\ B_\ell^{(4)} = Q_{\ell-1}^{(4)}(\mathcal{I} - \mathcal{K}_{\ell-1} + \mathcal{K}_\ell), \quad \ell = 2, 3, \dots \end{cases} \quad (3.21)$$

as generalizations of (3.18) and (3.19) respectively where $Q_\ell^{(j)}$ for $j = 3, 4$ is also an approximate inverse of $\mathcal{A}_\ell = (\mathcal{I} - \mathcal{K}_\ell)$ for $\ell = 1, 2, \dots$ and is defined by

$$\begin{aligned} Q_\ell^{(j)} &= \sum_{\mu=0}^{\gamma-1} (\mathcal{I} - B_\ell^{(j)} \mathcal{A}_\ell)^\mu B_\ell^{(j)} \\ &= [\mathcal{I} - (\mathcal{I} - B_\ell^{(j)} \mathcal{A}_\ell)^\gamma] \mathcal{A}_\ell^{-1}, \quad j = 3, 4; \quad \ell = 1, 2, \dots \end{aligned} \quad (3.22)$$

Refer to [58].

We are now in a position to investigate the convergence properties of MG-1 (rarely referred to in the literature) and MG-2.

THEOREM 3.2

Let $\xi_m^{(j)} = \|\mathcal{I} - B_m^{(j)} \mathcal{A}_m\|$ for $j = 1, 2, 3, 4$. Then

$$(1) \quad \xi_m^{(3)} \leq \xi_m^{(1)} + (\xi_{m-1}^{(3)})^\gamma (\xi_m^{(1)} + 1), \quad m = 2, 3, \dots; \quad (3.23)$$

$$(2) \quad \xi_m^{(4)} \leq \xi_m^{(2)} + (\xi_{m-1}^{(4)})^\gamma (\xi_m^{(2)} + 1), \quad m = 2, 3, \dots. \quad (3.24)$$

Proof. (1) To simplify, let us denote by

$$\begin{cases} \mathcal{U}_\ell = \mathcal{I} - B_\ell^{(1)} \mathcal{A}_\ell, \\ \mathcal{V}_\ell = \mathcal{I} - B_\ell^{(3)} \mathcal{A}_\ell. \end{cases} \quad (3.25)$$

From equation (3.18) we have $\mathcal{U}_\ell = \mathcal{I} - \mathcal{A}_{\ell-1}^{-1} \mathcal{A}_\ell$. Using this, (3.20) and (3.22) we have

$$\begin{aligned} \mathcal{V}_\ell &= \mathcal{I} - [\mathcal{I} - (\mathcal{I} - B_{\ell-1}^{(3)} \mathcal{A}_{\ell-1})^\gamma] \mathcal{A}_{\ell-1}^{-1} \mathcal{A}_\ell \\ &= \mathcal{U}_\ell + \mathcal{V}_{\ell-1}^\gamma (\mathcal{I} - \mathcal{U}_\ell). \end{aligned} \quad (3.26)$$

Taking norms, we obtain for $\ell = m$ the inequality (3.23).

(2) For the proof of (3.24), along similar lines, see [58]. \square

Theorem 3.2(1) has associated the convergence of MG-1 with that of TG-1 but has not actually proved it since $\xi_m^{(1)}$ may not go to zero as $m \rightarrow \infty$. In view of the condition (3.7), we can establish the convergence of MG-1 by showing that

$$\rho_m^{(3)} = \|(\mathcal{I} - B_m^{(3)} \mathcal{A}_m)^2\| \rightarrow 0 \text{ as } N_1 \rightarrow \infty.$$

The above result can be readily deduced from the following technical lemma (using (3.26)).

LEMMA 3.3

Let $\{\mathcal{U}_\ell\}_1^\infty$ and $\{\mathcal{V}_\ell\}_1^\infty$ be uniformly bounded linear operators as defined in (3.25), satisfying

$$\mathcal{V}_\ell = \mathcal{U}_\ell + \mathcal{V}_{\ell-1}^\gamma (\mathcal{I} - \mathcal{U}_\ell), \quad \ell \geq 2, \quad (3.27)$$

where $\gamma \geq 1$ is some integer constant. Then if $\gamma \geq 2$ and $\|\mathcal{U}_\ell^2\|, \|\mathcal{V}_1^2\| \rightarrow 0$ as $N_1 \rightarrow \infty$ (for any ℓ), we have

$$\|\mathcal{V}_\ell^2\| \rightarrow 0 \text{ as } N_1 \rightarrow \infty.$$

Proof. Square both sides of (3.27) and take norms. \square

Similar to the case of two grid methods, better convergence properties can be expected from MG-2 because of the additional residual smoothing step, though

MG-1 is roughly half as expensive as MG-2 per iteration. As mentioned earlier, many hybrid multigrid methods can be proposed (using ideas similar to TG-3) based upon a combination of MG-1 and MG-2; though they often require careful programming and tuning in order to make them more efficient than MG-2. Here we propose and test a simple three grid method which can be viewed as a combination of MG-1 and MG-2 (or TG-1 and TG-2) to be referred to as MG-3 and characterised by

$$\text{MG-3} \quad \begin{cases} B_1^{(5)} = (I - \mathcal{K}_1)^{-1} \\ B_{\ell-t}^{(5)} = I + B_1^{(5)} \mathcal{K}_{\ell-t} \\ B_t^{(5)} = Q_{\ell-t}^{(5)} \quad \ell = 2, 3, \dots \end{cases} \quad (3.28)$$

with $1 \leq t \leq \ell - 1$ (often $t = 1$ may be chosen) and (referring to (3.22))

$$Q_t^{(5)} = \sum_{\mu=0}^{\gamma-1} (I - B_{\ell-t}^{(5)} \mathcal{A}_t)^\mu B_t^{(5)}. \quad (3.29)$$

To present a convergence analysis analogous to those of MG-1 and MG-2, let us introduce similar to (3.25) the quantities :

$$\begin{cases} \mathcal{U}_t = I - \mathcal{A}_{\ell-t}^{-1} \mathcal{A}_t, \\ \mathcal{V}_t = I - B_{\ell-t}^{(5)} \mathcal{A}_{\ell-t}, \\ \mathcal{W}_t = I - B_t^{(5)} \mathcal{A}_t. \end{cases} \quad (3.30)$$

Then we have from (3.28)

$$\mathcal{V}_t = \mathcal{A}_1^{-1} (\mathcal{K}_{\ell-t} - \mathcal{K}_1) \mathcal{K}_{\ell-t}$$

and from (3.30)

$$\begin{aligned} \mathcal{W}_t &= I - [I - (I - B_{\ell-t}^{(5)} \mathcal{A}_{\ell-t})^\gamma] \mathcal{A}_{\ell-t}^{-1} \mathcal{A}_t \\ &= \mathcal{U}_t + \mathcal{V}_t^\gamma (I - \mathcal{U}_t). \end{aligned}$$

Further, noticing that $\|\mathcal{U}_t^2\| \rightarrow 0$ and $\|\mathcal{V}_t\| \rightarrow 0$ as $N_1 \rightarrow \infty$, we can prove the following result along the lines of the proof of Theorem 3.2 and Lemma 3.3.

THEOREM 3.4

Let $\xi_m^{(5)} = \|\mathcal{I} - B_m^{(5)}\mathcal{A}_m\|$ and $\rho_m^{(5)} = \|(\mathcal{I} - B_m^{(5)}\mathcal{A}_m)^2\|$. Then

$$(1) \quad \xi_m^{(5)} \leq \beta_{m-t,m}^I + (\beta_{1,m-t}^{II})^r(\beta_{m-t,m}^I + 1),$$

$$(2) \quad \rho_m^{(5)} \rightarrow 0 \text{ as } N_1 \rightarrow \infty,$$

where $\beta_{m-t,m}^I$ denotes the convergence rate of TG-1 based on levels $m-t$ and m , and $\beta_{1,m-t}^{II}$ the convergence rate of TG-2 based on levels 1 and $m-t$. □

3.5 Numerical experiments

In this section, we apply the iterative methods presented in §3.3–3.4 to two test problems. The first problem has the simple kernel $K(p, q) = \cos(\pi pq)$ and has been considered by many authors ([14], [52] and [58]). For this model problem with smooth kernel we demonstrate the fast convergence of all iterative methods -compared to the direct method and emphasize in particular the fact that two grid methods are performing as well as the multigrid methods.

The second problem arises from the boundary integral equation reformulation of the exterior acoustic problem with Dirichlet boundary condition, which will also be served as a model problem in the next chapter. This problem having a weakly singular complex valued kernel is perhaps more representative of practical situations, where the set up time could form a major part of the total computing time (see §3.6).

3.5.1 Test problem 1

The integral equation of the second kind is given by

$$u(p) - \lambda \int_0^1 \cos(\pi pq)u(q)dq = f(p), \quad p \in [0, 1] \quad (3.31)$$

where larger values of λ corresponds to a more difficult problem (less well-conditioned). We choose $f(p)$ such that the exact solution is $u(p) = e^p \cos(7p)$.

The operator \mathcal{K}_ℓ in (3.2) and (3.17) is defined via the Nyström method by

$$(\mathcal{K}_\ell u)(p) = \sum_{j=1}^{N_\ell} w_j K(p, q_j)u(p_j) \quad (3.32)$$

where \mathcal{K}_ℓ corresponds to discretizing \mathcal{K} with trapezium rule on a uniform mesh of size $h_\ell = 1/(N_\ell - 1)$.

3.5.2 Test problem 2 — the exterior Helmholtz equation

Here we consider the exterior Dirichlet boundary value problem for the Helmholtz equation (§1.2)

$$\begin{cases} (\nabla^2 + k^2)\phi(p) = 0, & p \in E, \\ \phi(p) = f(p), & p \in S, \\ \lim_{r \rightarrow \infty} r^{1/2} \left\{ \frac{\partial \phi}{\partial r} - ik\phi(p) \right\} = 0, & p \in E, \end{cases} \quad (3.33)$$

where $k = \omega/c$ is the acoustic wavenumber, ω the angular frequency of the sound source and c the speed of sound in the infinite acoustic medium E exterior to a smooth contour S in R^2 . We assume an integral representation for the solution $\phi(p)$ as a linear combination of the single and double layer Helmholtz potentials in the form (§1.3.1)

$$\phi(p) = (\mathcal{H}_k u)(p) = \int_S u(q) \left\{ \frac{\partial G_k}{\partial n_q}(p, q) - \eta G_k(p, q) \right\} dS_q, \quad p \in E \quad (3.34)$$

Table 3.1: Direct method for test problem 1 and test problem 2 (CPU times)

| Test problem 1 | | | Test problem 2 | | |
|----------------|--------|----------|----------------|--------|----------|
| N | Set up | Solution | N | Set up | Solution |
| 129 | 1.3 | 9.8 | 81 | 59.1 | 15.3 |
| 257 | 4.9 | 73.9 | 243 | 527.5 | 400.1 |
| 513 | 19.1 | 580.5 | | | |

where n_q denotes the unit normal to S at q directed into E . Imposing the Dirichlet boundary condition using appropriate jump properties of the potentials (Lemma 1.13) we obtain

$$u(p) + \int_S 2 \left\{ \frac{\partial G_k}{\partial n_q}(p, q) - \eta G_k(p, q) \right\} u(q) dS_q = f(p), \quad p \in S \quad (3.35)$$

where $G_k(p, q) = \frac{i}{4} H_0^{(1)}(k|p - q|)$ is the fundamental solution of the Helmholtz equation in R^2 and η is the coupling parameter. Here we choose S from a family of ellipses parameterized by $x = a \cos(t)$, $y = b \sin(t)$ with $t \in [0, 2\pi]$, where in particular $b/a = 1, 3$ and 4 are chosen, keeping the mean length of the axes $(a + b)/2$ equal to unity. We use $\eta = ik/2$ so as to minimize ('almost') the condition number of (3.35); refer to §1.4. In all cases we take $k = 5$ and the boundary conditions are chosen such that the problem is equivalent to the radiation problem having one point source at $(x, y) = (0.0, 0.5)$ with strength $(2 + 3i)$; refer to [10]. The numerical method is the iterated collocation method (§2.2) defined on piecewise polynomial space $S^{N,1}$ based on equally spaced subdivisions in $t \in [0, 2\pi]$ with the collocation points at mid-points of subintervals.

All numerical experiments for test problem 1 and test problem 2 are carried

out on PRIME 9950 and PRIME 850 respectively. In table 3.1, we give the CPU times (in seconds) required for solving both problems directly. Tables 3.2–3.3 give a comparison of the CPU times of iterative methods for test problem 1, whilst tables 3.4–3.5 are the CPU times for the second test problem. In tables 3.2–3.5 for iterative methods, we put the required numbers of iterations to achieve the tolerance of 10^{-4} in brackets and denote by ‘*’ divergence. As expected the direct method is the most expensive method of solution of (3.2). For the smooth test problem 1, the choice of the coarse grid is not very crucial, however for the practical test problem 2 the choice $N_n \approx (N_m)^{2/3}$ appears to be the most appropriate. All the two grid methods compare favourably with multigrid methods in reducing the total computing time.

3.6 Remarks and further discussion

We have presented multigrid type iterative methods for the numerical solution of the second kind integral equations, all of which perform considerably more efficiently than the direct solution of (3.2). The two grid methods and in particular our modification TG-3 perform satisfactorily and are also easy to implement. However, the multigrid methods interacting between three or more grid levels including MG-3 are more efficient than the two grid methods and in particular MG-2 is the most robust method.

As can be seen from results in table 3.1 (in particular for the test problem 2), the set up time can form a major part of the total computing time. We observe that in multigrid type methods (and in the conjugate gradient method of the next Chapter) the matrix K_ℓ from (3.2) is only required in calculating results

of matrix vector multiplications. However matrix vector multiplications may be carried out accurately without the explicit knowledge of all the elements of K_ℓ since

$$K_\ell u_\ell = [(\mathcal{K}u)(p_1), (\mathcal{K}u)(p_2), \dots, (\mathcal{K}u)(p_{N_\ell})]^T.$$

This seems to suggest that all that is needed is some efficient method of evaluating accurately the functional $(\mathcal{K}u)(p)$ at all $G[\ell]$ points. Such a method will reduce the set up time as well as the solution time of iterative methods. This idea has been exploited by Hackbusch and Nowak in their recent work [53], [54] and [76], promising to reduce the complexity of a matrix vector multiplication from $O(N_\ell^2)$ to $O(N_\ell \log^{d+2} N_\ell)$ where d is the dimension associated with the integral boundary; (*i.e.* $d = 2$ for 2D and $d = 3$ for 3D).

Their method, referred to as the *panel clustering*, is based on the assumption that the kernel of the integral operator, $K(p, q)$, has a finite series expansion or an accurate finite series approximation at the 'far field' (*i.e.* $|p - q|$ large). We now give a brief description of the panel clustering method. Following (3.1), let us define a linear integral operator by

$$(\mathcal{K}u)(p) = \int_S K(p, q)u(q)dS_q, \quad (3.36)$$

where $S \subset R^d$ is a $(d-1)$ dimensional manifold. For a partition of S , $S = \bigcup_{i=1}^n \Delta_i$, by n panels (elements²) as in (2.23), iterative methods with the collocation approximation require the values of the quantities

$$(\mathcal{K}u_n)(p) = \sum_{i=1}^n \int_{\Delta_i} K(p, q)u_n(q)dS_q \quad (3.37)$$

²Here our panel method is as introduced in §2.1. There is no assumption on surface approximation for the moment.

at all $G[n]$ points in S . We now seek an alternative representation for (3.37). For each point $p \in G[n]$, we are able to represent the boundary S by a combination of panels (Δ) and clusters (T)

$$S = \Delta_1 \cup \cdots \cup \Delta_\tau \cup T_1 \cup \cdots \cup T_c, \quad (3.38)$$

where each cluster T is a union of several panels (Δ), $\tau = O(1)$ and $c = O(\log^{d+2} n)$. In (3.38), clusters $\{T_j\}_1^c$ are said to be in the 'far field' with respect to p , by requiring that $|p - q|$ is sufficiently large ($q \in T_j$, $j = 1, \dots, c$); while panels $\{\Delta_i\}_1^\tau$ are said to be in the 'near field' accordingly. Hence (3.37) can be replaced by

$$(\mathcal{K}u_n)(p) = \sum_{i=1}^{\tau} \int_{\Delta_i} K(p, q)u_n(q)dS_q + \sum_{j=1}^c \int_{T_j} K(p, q)u_n(q)dS_q. \quad (3.39)$$

In T_j — the 'far field', the kernel $K(p, q)$ has a finite series expansion or an accurate finite series approximation as assumed

$$K(p, q) \doteq \sum_{i \in I_n} K_i(p; q_j)\Phi_i(q) \quad (3.40)$$

where all $\Phi_i(q)$ are independent of p and I_n is an index set indicating the order of the expansion and q_j is the center of cluster T_j . Now we may substitute (3.40) for $j = 1, \dots, c$ into (3.39), giving

$$(\mathcal{K}u_n)(p) = \sum_{i=1}^{\tau} \int_{\Delta_i} K(p, q)u_n(q)dS_q + \sum_{j=1}^c \sum_{m \in I_n} K_m(p; q_j) \int_{T_j} \Phi_m(q)u_n(q)dS_q. \quad (3.41)$$

Since the quantities

$$J_{T_j}^m = \int_{T_j} \Phi_m(q)u_n(q)dS_q, \quad m \in I_n, \quad j = 1, \dots, c \quad (3.42)$$

are independent of p , they can be computed first and once only for a given u_n .

It can be shown that the work of computing all possible $J_{T_j}^m$ for all $p \in G[n]$ is of

order $O(n)$ operations. The first sum in (3.41) corresponding to the 'near field' $\Delta_1 \cup \dots \cup \Delta_r$ will be evaluated accurately, requiring the work of $O(1)$ operations for each $p \in G[n]$. Therefore from (3.42), evaluating

$$(\mathcal{K}u_n)(p) = \sum_{i=1}^r \int_{\Delta_i} K(p, q)u_n(q)dS_q + \sum_{j=1}^c \sum_{m \in I_n} K_m(p; q_j) \cdot J_{T_j}^m, \quad (3.43)$$

for all $p \in G[n]$ will require roughly $O(nc)$ i.e. $O(N_n \log^{d+2} N_n)$ operations. In the mean time the storage is also reduced to that of a similar order. We refer the reader to [54] and the references therein for more details.

Such works on reducing the set up time may improve most iterative methods substantially. But the present method is not readily applicable to many practical problems (even to some model problems). Apart from the complex programming, the main problem lies in the unavailability of an efficient series expansion such as (3.40). In [54], the expansion is obtained from the Taylor series, which requires the use of higher derivatives of a function. As is well known, it is generally not trivial to implement numerical differentiation accurately. In [54], only the case of weakly singular kernels is considered.

Another approach has been studied by Rokhlin [84] in solving the Laplace equation, where the solution is represented by a double layer potential. The integral equation hence obtained is discretized by the Nyström method based on the trapezium rule. The approach suggested there is highly complicated, restrictive and is not as competitive as that of Hackbusch and Nowak; see [76]. It appears that much further work is still required to develop practical schemes to improve the existing iterative methods. We refer also to [94] for a general and prospective exposition.

Table 3.2: Two grid methods for test problem 1 (CPU times)

| λ | N_m | N_n | TG-1 | TG-2 | TG-3 | Set up | | |
|-----------|-------|----------|----------|----------|----------|---------|---------|-----|
| 1 | 129 | 9 | 0.6 (2) | 1.2 (2) | 0.7 (2) | 1.3 | | |
| | | 17 | 0.7 (2) | 1.3 (2) | 0.7 (2) | 1.3 | | |
| | | 33 | 1.0 (2) | 1.5 (2) | 1.0 (2) | 1.4 | | |
| | | 65 | 2.1 (2) | 2.9 (2) | 2.4 (2) | 1.5 | | |
| | 257 | 17 | 2.7 (2) | 4.9 (2) | 2.7 (2) | 5.0 | | |
| | | 33 | 3.1 (2) | 5.2 (2) | 3.0 (2) | 5.2 | | |
| | | 65 | 4.7 (2) | 6.8 (2) | 4.6 (2) | 5.3 | | |
| | | 129 | 12.3 (1) | 12.9 (1) | 11.8 (1) | 6.0 | | |
| | | 129 | 9 | 0.9 (3) | 1.7 (3) | 1.0 (3) | 1.3 | |
| | | 129 | 17 | 0.7 (2) | 1.2 (2) | 0.8 (2) | 1.3 | |
| 10 | 129 | 33 | 1.0 (2) | 1.5 (2) | 1.0 (2) | 1.4 | | |
| | | 65 | 2.5 (2) | 2.9 (2) | 2.4 (2) | 1.5 | | |
| | | 257 | 17 | 2.7 (2) | 4.9 (2) | 2.7 (2) | 5.0 | |
| | | 33 | 3.1 (2) | 5.2 (2) | 3.0 (2) | 5.1 | | |
| | 257 | 65 | 4.7 (2) | 6.8 (2) | 4.6 (2) | 5.3 | | |
| | | 129 | 12.3 (1) | 12.9 (1) | 11.8 (1) | 6.0 | | |
| | | 100 | 129 | 9 | 1.9 (6) | * | 1.9 (6) | 1.3 |
| | | | 17 | 1.1 (3) | 2.4 (4) | 1.1 (3) | 1.3 | |
| | | | 33 | 1.0 (2) | 2.1 (3) | 1.0 (2) | 1.4 | |
| | | | 65 | 2.5 (2) | 2.9 (2) | 2.4 (2) | 1.5 | |
| 257 | 17 | 4.0 (3) | 9.9 (4) | 3.9 (3) | 5.0 | | | |
| | 33 | 3.1 (2) | 7.8 (3) | 3.0 (2) | 5.1 | | | |
| | 65 | 4.7 (2) | 6.8 (2) | 4.6 (2) | 5.3 | | | |
| | 129 | 14.3 (2) | 15.9 (2) | 13.7 (2) | 6.0 | | | |

Table 3.3: Multigrid methods for test problem 1 (CPU times)

| λ | N_m | m | N_1 | MG-1 | MG-2 | MG-3 | Set up |
|-----------|-------|-----|-------|---------|-----------|----------|--------|
| 1 | 129 | 5 | 9 | 2.0 (2) | 1.6 (1) | 1.7 (2) | 2.1 |
| | | 4 | 17 | 1.9 (2) | 1.5 (1) | 1.8 (2) | 2.1 |
| | | 3 | 33 | 1.8 (2) | 1.5 (1) | 2.0 (2) | 2.1 |
| | 257 | 5 | 17 | 5.0 (1) | 6.1 (1) | 4.5 (1) | 8.0 |
| | | 4 | 33 | 4.9 (1) | 5.8 (1) | 4.8 (1) | 8.0 |
| | | 3 | 65 | 5.7 (1) | 6.3 (1) | 6.4 (1) | 8.0 |
| 10 | 129 | 5 | 9 | 2.6 (3) | 2.9 (2) | 2.3 (3) | 2.1 |
| | | 4 | 17 | 1.9 (2) | 2.4 (2) | 1.8 (2) | 2.1 |
| | | 3 | 33 | 1.8 (2) | 2.2 (2) | 2.2 (2) | 2.1 |
| | 257 | 5 | 17 | 7.5 (2) | 9.6 (2) | 6.9 (2) | 8.0 |
| | | 4 | 33 | 4.9 (1) | 9.0 (2) | 4.8 (1) | 8.0 |
| | | 3 | 65 | 5.7 (1) | 15.9 (1) | 6.3 (1) | 8.0 |
| 100 | 129 | 5 | 9 | * | * | * | 2.1 |
| | | 4 | 17 | 5.0 (3) | 10.7 (13) | * | 2.1 |
| | | 3 | 33 | 1.8 (2) | 2.9 (3) | 3.8 (5) | 2.1 |
| | 257 | 5 | 17 | * | * | * | 8.0 |
| | | 4 | 33 | 9.6 (3) | 12.1 (3) | 14.2 (5) | 8.0 |
| | | * | 65 | 7.9 (2) | 9.1 (2) | 11.4 (3) | 8.0 |

Table 3.4: Two grid methods for test problem 2 (CPU times)

| b/a | N_m | N_n | TG-1 | TG-2 | TG-3 | |
|-------|-------|-------|------------|------------|------------|----------|
| 1 | 81 | 9 | 22.7 (19) | 25.1 (10) | 23.1 (16) | |
| | | 27 | 6.7 (4) | 9.5 (3) | 8.2 (3) | |
| | 243 | 9 | 172.5 (19) | 194.3 (10) | 181.0 (16) | |
| | | 27 | 41.6 (4) | 68.8 (3) | 48.6 (3) | |
| | | 81 | 9 | 44.3 (2) | 76.9 (2) | 48.9 (2) |
| | | | 27 | | | |
| 3 | 81 | 9 | 46.5 (39) | 46.4 (31) | 48.7 (31) | |
| | | 27 | 10.3 (6) | 12.5 (4) | 11.2 (5) | |
| | 243 | 9 | 363.7 (40) | 398.9 (20) | 399.1 (32) | |
| | | 27 | 61.7 (6) | 85.5 (4) | 67.0 (5) | |
| | | 81 | 9 | 59.3 (3) | 72.9 (2) | 63.3 (3) |
| | | | 27 | | | |
| 4 | 81 | 9 | 84.5 (72) | 71.6 (27) | 38.3 (13) | |
| | | 27 | 11.0 (7) | 15.3 (5) | 12.5 (6) | |
| | 243 | 9 | 708.5 (78) | 566.8 (29) | 324.3 (13) | |
| | | 27 | 82.2 (8) | 106.7 (5) | 85.4 (7) | |
| | | 81 | 9 | 57.2 (3) | 82.4 (2) | 62.6 (3) |
| | | | 27 | | | |

Table 3.5: Multigrid methods for test problem 2 (CPU times)

| b/a | N_m | m | N_1 | MG-1 | MG-2 | MG-3 |
|-------|-------|-----|-------|-----------|----------|-----------|
| 1 | 81 | 3 | 9 | 11.2 (12) | 5.9 (5) | 7.8 (6) |
| | 243 | 4 | 9 | 65.4 (8) | 25.5 (2) | 81.4 (7) |
| | | 3 | 27 | 28.6 (3) | 26.1 (2) | 27.0 (2) |
| 3 | 81 | 3 | 9 | 21.5 (24) | 8.2 (7) | 13.9 (12) |
| | 243 | 3 | 27 | 45.1 (5) | 37.1 (3) | 35.6 (3) |
| 4 | 81 | 3 | 9 | 34.1 (38) | 8.9 (8) | 19.2 (14) |
| | 243 | 3 | 27 | 43.2 (5) | 34.4 (3) | 44.3 (4) |

Chapter 4

Conjugate Gradient Method for Smooth Integral Equations

For the numerical solution of an integral equation of the second kind, we have discussed in the last Chapter a class of multigrid type iterative methods that interact between two or more grids by referring to the underlying integral equation. These methods are in general efficient, but they all involve choosing appropriate parameters (such as ratios between step sizes of different grids and the cycling pattern) as well as requiring careful and complex programming to ensure fast convergence. Here in this chapter, we present the easily programmable conjugate gradient method (CGM), which is free from problem dependent parameters, always converging and above all superior to direct methods. We then prove the fast convergence of the CGM for solving linear systems arising from the discretization of integral equations with a compact operator. In fact, as a linear system solver, the use of CGM is not just limited to those arising from the discretization of integral equations of compact operators. In Chapter 6, we shall demonstrate its

fast convergence even when applied to a class of non-compact operator equations.

4.1 Introduction

Recall the setting of §3.1, where a second kind integral equation is defined in operator notation by

$$(\mathcal{I} - \mathcal{K})u = f(p), \quad p \in S, \quad (4.1)$$

and its approximate equation on grid $G[\ell]$ is given by

$$(\mathcal{I} - \mathcal{K}_\ell)u_\ell = f. \quad (4.2)$$

The solution of (4.2) is determined via the Nyström interpolation

$$u_\ell(p) := f + \mathcal{K}_\ell u_\ell, \quad p \in S, \quad (4.3)$$

after the solution vector $\underline{u}_\ell = \{(u_\ell)(p_1), (u_\ell)(p_2), \dots, (u_\ell)(p_{N_\ell})\}^T$ is found by solving the following linear system

$$A_\ell \underline{u}_\ell = \underline{f}, \quad A_\ell = I - K_\ell, \quad (4.4)$$

with $\underline{f} = [f(p_1), f(p_2), \dots, f(p_{N_\ell})]^T$. Here we shall concentrate on solving (4.4) as a linear system of size $N_\ell \times N_\ell$, whilst iterative methods from Chapter 3 have been aimed at (4.2).

As noted in [27], the application of simple iterative methods ([16, §8.9] and [46, Ch.10]) such as the successive overrelaxation (SOR) to (4.4) runs into difficulty in ensuring the convergence. So Burton [27] suggested the use of a simple conjugate gradient method for solving exterior acoustic problems and observed the fast convergence. However for solving matrix equations with complex elements several

variants of the conjugate gradient method can be found in the literature; (see [85] for example). Here we shall adopt the version as used in [27] and provide it with a convergence analysis.

This chapter is divided into several sections. In §4.2, we state and prove our main results concerning the rate of convergence of the conjugate gradient method for matrices possessing eigenvalue clustering properties. In §4.3, we discuss the spectral properties of compact integral operators, leading to the application of the theory of §4.2 with some emphasis on solving Helmholtz equations. Some numerical results for the 2 and 3 dimensional exterior acoustic problems are presented in §4.4.

4.2 The conjugate gradient method

The conjugate gradient (CG) method for solving a $n \times n$ linear system

$$A\underline{x} = \underline{b} \tag{4.5}$$

where A is symmetric and positive definite, is due to Hestenes and Steifel [59]. The method is based on the fact that, \underline{x}^* is the solution of (4.5) iff it minimizes the quadratic functional

$$\phi(\underline{x}) = \frac{1}{2}\underline{x}^T A \underline{x} - \underline{x}^T \underline{b}. \tag{4.6}$$

Strictly speaking, the CG method is a direct method, as in the absence of any rounding errors it would yield the exact solution \underline{x}^* in at most n steps. Here we shall show that for a large class of problems arising from discretization of second kind integral equations a sufficiently accurate solution can be obtained in μ steps say, where μ is independent of n but depends on the characteristics of the problem

and the accuracy requirement. We refer the reader to [46, Ch.10] and also to the later part of this section for examples of CG algorithms.

An important property of the CG method used in deriving error bounds for the method is the analogy between CG iterations and a polynomial curve fitting; see [59] and [62]. If we define the A-norm (energy norm) of a vector $\underline{x} \in R^n$ by $\|\underline{x}\|_A = \underline{x}^T A \underline{x}$, it can be shown that if $\hat{\underline{x}}$ is an approximation to \underline{x}^* , then

$$E(\hat{\underline{x}}) = 2[\phi(\hat{\underline{x}}) - \phi(\underline{x}^*)] = \underline{r}^T A^{-1} \underline{r} = \|\hat{\underline{x}} - \underline{x}^*\|_A \quad (4.7)$$

where $\underline{r} = \underline{b} - A\hat{\underline{x}}$ is the residual vector and hence $E(\cdot)$ is a measure of the error. Further, let us denote the eigenvalues of A by $\{\lambda_i\}$ with corresponding normalised eigenvectors $\{\underline{q}_i\}$, $i = 1, 2, \dots, n$. If $\underline{x}^{(k)}$ is the approximation to \underline{x}^* after k steps of the CG method and the initial residual vector $\underline{r}_0 = \underline{b} - A\underline{x}^{(0)} = \sum s_i \underline{q}_i$, it can be shown that

$$E(\underline{x}^{(k)}) = \sum_{i=1}^n w_i [p_k^*(\lambda_i)]^2 \quad (4.8)$$

where $w_i = s_i^2 / \lambda_i$ and $p_k^*(\lambda)$ is the k -th degree polynomial which satisfies $p_k^*(0) = 1$ and is the *least square fit* to zero at the points λ_i with weights w_i , i.e. p_k^* minimises the functional $\sum_{i=1}^n w_i [p_k(\lambda_i)]^2$ among all the k -th degree polynomials satisfying $p_k(0) = 1$. Clearly, if A has m ($m \leq n$) distinct eigenvalues, then $E(\underline{x}^{(m)}) = 0$, i.e. $\underline{x}^{(m)} = \underline{x}^*$ in the absence of rounding errors. This property for an algorithm is usually called the fixed step termination. We now state and prove some results concerning the efficiency of the CG method, in particular when the matrix has some desirable clustering properties; (refer to the next section for examples).

THEOREM 4.1

Let A be an $n \times n$ symmetric positive definite matrix with eigenvalues $0 < \lambda_1 \leq$

$\lambda_2 \leq \dots \leq \lambda_n$, then after r iterations of the CG method applied to $A\underline{x} = \underline{b}$, the approximation $\underline{x}^{(r)}$ satisfies

$$\frac{E(\underline{x}^{(r)})}{E(\underline{x}^{(0)})} \leq 4[\sigma(C)]^r, \quad \sigma(C) = \left[\frac{\sqrt{C} - 1}{\sqrt{C} + 1} \right]^2 \quad (4.9)$$

where $C = \lambda_n/\lambda_1$ is the 2-norm condition number of A .

Proof. Refer to [38] for a detailed proof. Here we only give a brief outline in order to motivate the proof of next theorem. Let us construct an r -th degree polynomial $p_r(\lambda)$ by

$$p_r(\lambda) = T_r \left[\frac{\lambda_n + \lambda_1 - 2\lambda}{\lambda_n - \lambda_1} \right] / T_r \left[\frac{\lambda_n + \lambda_1}{\lambda_n - \lambda_1} \right],$$

to be used in comparison to the least square polynomial fit p_r^* to give an error bound, where $T_r(y) = \cos(r \cos^{-1} y) = [(y + \sqrt{y^2 - 1})^r + (y - \sqrt{y^2 - 1})^r]/2$ is the r -th order Chebyshev polynomial of the first kind ([43]). Therefore, we have

$$E(\underline{x}^{(r)}) \leq \sum_1^n w_i [p_r(\lambda_i)]^2.$$

Following the relations (see [43] and [83])

$$\begin{cases} |T_r(y)| \leq 1 & \text{if } |y| \leq 1, \\ \left[T_r \left(\frac{\lambda_n + \lambda_1}{\lambda_n - \lambda_1} \right) \right]^{-2} = 4 \frac{\sigma^r}{(1 + \sigma^r)^2}, \end{cases} \quad (4.10)$$

where $\sigma = \left[\frac{\sqrt{C} - 1}{\sqrt{C} + 1} \right]^2$, we obtain

$$\frac{E(\underline{x}^{(r)})}{E(\underline{x}^{(0)})} \leq 4 \frac{\sigma^r}{(1 + \sigma^r)^2} \quad (4.11)$$

$$\leq 4\sigma^r. \quad (4.12)$$

Thus the proof is complete. \square

It can be seen from (4.9) that $\sigma(C) = \sigma$ approximates the convergence rate of the CG method. See also [20]. Clearly (4.11) may provide a sharper bound but

(4.9) i.e. (4.12) is traditionally referred to in most literature. Here we follow the tradition, while bearing in mind that all theoretical error bounds so generated may be sharpened.

It follows from (4.9) that for well-conditioned problems we can expect a fast convergence. In particular if all the eigenvalues of A are clustered around one point then $C \approx 1$ and hence $\sigma(C)$ will be very small, indicating that perhaps one or two CG iterations may yield sufficiently accurate solutions. In general for many cases of practical interests arising from boundary element methods (see [3] and [20]) the spectrum of A , $\Sigma(A)$, includes a few eigenvalues either side of a main cluster region. This is due to the desirable eigenvalue clustering property of compact operators; (see the next section). We shall now improve the estimate in (4.9) by proving an important result concerning the order of convergence of the CG method for matrices with such eigenvalue distributions.

THEOREM 4.2

Let A be an $n \times n$ symmetric positive definite matrix, where most of its eigenvalues cluster in a region $[\alpha, \beta]$. To be precise, we assume $0 < \lambda_i \leq \alpha$ for $i = 1, 2, \dots, \ell$; $\lambda_i > \beta$ for $i = n - m + 1, \dots, n$ while the remaining $n - m - \ell$ eigenvalues are inside $[\alpha, \beta]$. Then after $\mu = \sum_{i=1}^{\ell} t_i + m + r$ steps of the CG method applied to $A\underline{x} = \underline{b}$, the approximation $\underline{x}^{(\mu)}$ satisfies

$$\frac{E(\underline{x}^{(\mu)})}{E(\underline{x}^{(0)})} \leq 4[\sigma(\bar{C})]^r, \quad \sigma(\bar{C}) = \left[\frac{\sqrt{\bar{C}} - 1}{\sqrt{\bar{C}} + 1} \right]^2, \quad (4.13)$$

where $\bar{C} = \beta/\alpha$ and

$$t_i = \begin{cases} 1, & \text{for } \lambda_i \geq \frac{\beta}{2}, \\ \lfloor \frac{\pi}{2 \cos^{-1}(1 - 2\lambda_i/\beta)} \rfloor + 1, & \text{otherwise,} \end{cases} \quad (4.14)$$

and $\lfloor \cdot \rfloor$ denotes the integer part of a real number.

Proof. In view of equation (4.8) we aim to construct $p_\mu(\lambda)$ which satisfies $p_\mu(0) = 1$ and takes sufficiently small values in modulus at the eigenvalues of A . Consider

$$p_\mu(\lambda) = U_t(\lambda) \cdot V_r(\lambda) \cdot W_m(\lambda) \quad (4.15)$$

where U_t , V_r and W_m are polynomials of degree of $t = \sum_1^\ell t_i$, r and m respectively and are given by

$$U_t(\lambda) = \prod_{i=1}^t \frac{T_{t_i} \left[\frac{(\beta-\lambda) \cos(\frac{\pi}{2t_i}) + (\lambda_i - \lambda)}{\beta - \lambda_i} \right]}{T_{t_i} \left[\frac{\beta \cos(\frac{\pi}{2t_i}) + \lambda_i}{\beta - \lambda_i} \right]}, \quad (4.16)$$

$$V_r(\lambda) = T_r \left[\frac{\beta + \alpha - 2\lambda}{\beta - \alpha} \right] / T_r \left[\frac{\beta + \alpha}{\beta - \alpha} \right], \quad (4.17)$$

$$W_m(\lambda) = \prod_{i=n-m+1}^n \left[1 - \frac{\lambda}{\lambda_i} \right]. \quad (4.18)$$

Using the relation in (4.10) and the condition (4.14), we have for (4.16) that

$$|U_t(\lambda)| \leq 1 \quad \text{for } \lambda \in [\alpha, \beta]. \quad (4.19)$$

Furthermore, it can be easily shown that $U_t(\lambda_i) = 0$ for $i = 1, 2, \dots, \ell$ and $U_t(0) = 1$. As for (4.17), clearly $V_r(0) = 1$ and similar to the proof of Theorem 4.1 it can be shown that

$$|V_r(\lambda)| \leq 2 \left[\frac{\sqrt{C} - 1}{\sqrt{C} + 1} \right]^r \quad \text{for } \lambda \in [\alpha, \beta]. \quad (4.20)$$

For (4.18) it is easy to see that $W_m(0) = 1$ and $W_m(\lambda_i) = 0$ for $i = n-m+1, \dots, n$, and that

$$|W_m(\lambda)| = \left| \prod_{i=n-m+1}^n \frac{\lambda_i - \lambda}{\lambda_i} \right| \leq 1 \quad \text{for } \lambda \in [\alpha, \beta]. \quad (4.21)$$

It now follows from (4.8) and (4.15)-(4.21) that

$$E(\underline{x}^{(\mu)}) \leq \sum_{i=1}^n w_i [p_\mu(\lambda_i)]^2 \leq \max_{\lambda \in [\alpha, \beta]} |p_\mu(\lambda)|^2 \cdot E(\underline{x}^{(0)}), \quad (4.22)$$

which completes the proof. \square

Remarks

- (a). In Theorem 4.2, we proved that any iteration of the CG method, after $\mu^* = \sum_1^{\ell} t_i + m \geq \ell + m$ steps, can reduce the error substantially provided $\bar{C} = \beta/\alpha \simeq 1$, as $\sigma(\bar{C})$ would be close to zero. Clearly choosing a smaller cluster region $[\alpha, \beta]$ would in general imply larger values for ℓ and m and therefore, may not necessarily give a sharper error bound. The number of iterations required to achieve a certain degree of accuracy depends crucially on ℓ , m and $\bar{C} = \beta/\alpha$. Fortunately in the case of second kind integral equations with compact operators the values of ℓ , m and \bar{C} are generally small, hence implying fast convergence from (4.13). Notice that if we choose $\ell = m = 0$, Theorem 4.2 reduces to Theorem 4.1.
- (b). The number of iterations required to obtain the error bound (4.13) is independent of n , indicating that if we were to solve a family of linear systems of different order, then a "fixed" number of the iterations of the CG method can be expected to yield similar order of accuracy, provided that the cluster regions are the same and ℓ and m are the same. This fact will be exploited in §4.3 and §4.4.
- (c). In general, linear systems arising from boundary element methods are complex and non-Hermitian (*i.e.* $A \neq A^*$). We can easily show that all results in the section for real symmetric and positive definite matrices A are also valid for complex Hermitian positive definite matrices A , provided that a real transpose vector \underline{y}^T is replaced by a complex transpose conjugate \underline{y}^* and that the A -norm for a complex vector \underline{y} is defined by $\|\underline{y}\|_A = \underline{y}^* A \underline{y}$. Therefore for the complex linear system $A \underline{x} = \underline{b}$, the CG method may be

applied to the equivalent problem (refer to [27] and [85])

$$B\underline{y} = \underline{b} \quad (4.23)$$

where $B = AA^*$ and $\underline{x} = A^*\underline{y}$. The matrix B is not formed explicitly as it is only required in matrix-vector multiplications such as $\underline{v} = B\underline{u}$, which is the most expensive part of a CG iteration and is suitable for calculations on vector and parallel processors; refer to [8], [16, p.571] and the CG algorithm below. The 2-norm condition number of $B = AA^*$ is the square of that of A , which is why the CG method is rarely used for solving the normal equation (4.23); see [85]. In our application area however the condition number of A and hence that of B are generally small and, more importantly, the clustering property of B can guarantee fast convergence (Theorem 4.2).

- (d). If the eigenvalues of A cluster around μ^* say, we may expect the eigenvalues of AA^* to cluster around $|\mu^*|^2$, as is indeed the case in all our numerical calculations of §4.4. In particular if A is obtained as a result of discretizing the second kind operator $(\lambda I - \mathcal{K})$ where \mathcal{K} is compact, it is easy to show that λ is the only possible point of eigenvalue accumulation. We leave further discussion to the next section.

Finally in this section, we describe a CG algorithm for solving $A\underline{x} = \underline{b}$ via $AA^*\underline{y} = \underline{b}$ for a non-singular complex and non-Hermitian matrix A and an arbitrary right hand side complex vector \underline{b} .

ALGORITHM – Conjugate gradients :

- 0) Set $\underline{x} := 0$, $\underline{p} := 0$, $\underline{r} := \underline{b}$, $c_1 := 1$ and input TOL;
- 1) Compute $c_2 := \underline{r}^*\underline{r}$, $E := \sqrt{c_2}$;

- 2) If $E/\|b\|_2 \leq \text{TOL}$, then exit with solution \underline{x} ;
- 3) Compute $\beta := c_2/c_1$;
- 4) Assign $c_1 := c_2$;
- 5) Compute $\underline{p} := \underline{r} + \beta \underline{p}$;
- 6) Compute $\underline{q} := A^* \underline{p}$;
- 7) Compute $\alpha := c_2/\underline{q}^* \underline{q}$;
- 8) Compute $\underline{x} := \underline{x} + \alpha \underline{q}$, $\underline{r} := \underline{r} - \alpha A \underline{q}$;
- 9) Return to step 1) and continue. □

4.3 Spectral properties of compact operators

In this section, we shall apply the results of the last section to the solution of second kind integral equations. Particularly relevant and important is the fact that, for $S \in C^2$, many of the integral operators $\int_S K(p, q) \sigma(q) dS_q$ arising in the boundary integral formulations of elliptic PDE's (see Chapter 1) are compact. The following spectral property of compact operators (refer to [60] and [75]) is precisely the one which ensures the fast convergence of the conjugate gradient (CG) method (refer to Theorem 4.2).

THEOREM 4.3

Let \mathcal{K} be a compact operator on a Hilbert space $(X, (\cdot, \cdot)_X)$. Then $\Sigma(\mathcal{K})$, the eigenvalue spectrum of \mathcal{K} , is (at most) countably infinite and $\lambda = 0$ is the only possible point of accumulation. □

Provided that \mathcal{K} in (4.1) is compact, $\lambda = 1$ is the only point of accumulation of $(\mathcal{I} - \mathcal{K})$. It follows from the Fredholm-Riesz theory that, provided $1 \notin \Sigma(\mathcal{K})$, the equation (4.1) has a unique solution (see Chapter 1). However in practice, if $\text{dist}(1, \Sigma(\mathcal{K}))$ is small, then (4.1) suffers from ill-conditioning which makes it difficult to obtain accurate approximations u_ℓ to solution u ; see [10] and [14].

From Theorem 4.3 and [11, §4.5], we know that eigenvalues of the approximate operator \mathcal{K}_ℓ converge to those of \mathcal{K} and that these eigenvalues also have one possible point of accumulation (zero) independent of the size N_ℓ , provided that \mathcal{K} is compact. As also known from Theorem 1.12, integral operators arising from reformulations of Helmholtz equations are compact so the efficiency of the CG method is ensured for their numerical solutions (Theorem 4.2). In the rest of the section, we first illustrate the clustering property of compact operators for the case of a simple geometry S and then show the similar property exhibited by discrete normal operators in order to justify the use of the CG algorithm of last section as a fast solver.

Let us for the moment concentrate on the 3D exterior Helmholtz problem where the structure of the boundary S is a unit sphere (refer to (4.1) and Chapter 1). The following result from [3] gives the eigenvalues of the relevant integral operators.

THEOREM 4.4

The eigenvalues of the operator $(\frac{1}{2}\mathcal{I} + M_k^T - \eta L_k)$, for the Dirichlet problem, are given by

$$\lambda_n(k) = -ikh_n(k)\{\eta j_n(k) + j'_n(k)\}, \quad n = 0, 1, 2, \dots \quad (4.24)$$

and the eigenvalues of the operator $(-\frac{1}{2}\mathcal{I} + M_k + \eta N_k)$, for the Neumann problem, are given by

$$\mu_n(k) = -ik^2 h'_n(k) \{j_n(k) + \eta j'_n(k)\}, \quad n = 0, 1, 2, \dots \quad (4.25)$$

whilst, the eigenvalues of the regularised operator $-\frac{1}{2}\mathcal{I} + M_k + \eta[L_0(N_k - N_0) + M_0^2 - \frac{I}{4}]$ for the Neumann problem, are given by

$$\delta_n(k) = ik^2 h_n(k) \{j_n(k) + \frac{\eta k}{2n+1} j'_n(k)\}, \quad n = 0, 1, 2, \dots \quad (4.26)$$

where h_n denotes the spherical Hankel function of the first kind and j_n denotes the spherical Bessel-function of order n ; (see [3] and [97]). \square

In order to observe more clearly the characteristics of $\lambda_n(k)$ and $\mu_n(k)$, let us look at the potential theoretic case $k = 0$, where (4.24), (4.25) and (4.26) respectively reduce to (refer to [3])

$$\lambda_n = \frac{1}{2} - \frac{1+2\eta}{2(2n+1)} \quad n = 0, 1, 2, \dots, \quad (4.27)$$

$$\mu_n = -\frac{1}{2} - \frac{1+2\eta n(n+1)}{2(2n+1)} \quad n = 0, 1, 2, \dots, \quad (4.28)$$

$$\delta_n = -\left(\frac{1}{2} + \frac{\eta}{4}\right) - \frac{2(2n+1) - \eta}{4(2n+1)^2}, \quad n = 0, 1, 2, \dots, \quad (4.29)$$

where asymptotically both λ_n and δ_n , obviously bounded, accumulate at one point as expected for compact operators¹.

Now we consider the problem of solving the matrix equation $A\underline{x} = \underline{b}$ via the normal equation $AA^*\underline{y} = \underline{b}$ with $A = I - K_\ell$. The clustering property of AA^* will follow that of A . In fact, we can show that AA^* is the matrix associated with operator $(\mathcal{I} - \mathcal{K}_\ell)(\mathcal{I} - \mathcal{K}_\ell)^*$, which approximates the operator

¹We do not expect μ_n to have the similar asymptotic behaviour since the operator N_0 is non-compact.

$(\mathcal{I} - \mathcal{K})(\mathcal{I} - \mathcal{K})^* = \mathcal{I} - \mathcal{K} - \mathcal{K}^* - \mathcal{K}\mathcal{K}^*$. Note that $\mathcal{K} + \mathcal{K}^* + \mathcal{K}\mathcal{K}^*$ is also a compact operator if \mathcal{K} is compact; (see Theorem 1.4). Hence the eigenvalue accumulation point for AA^* is still 1. If \mathcal{K} is a normal operator, that is, if $\mathcal{K}^*\mathcal{K} = \mathcal{K}\mathcal{K}^*$, then $\lambda_i(AA^*) = \lambda_i(A^*A) = |\lambda_i(A)|^2$ where λ_i denotes the i -th eigenvalue of its argument. We note in passing that for integral equations of the form (2.8) for example we can show that if the kernel of the integral operator \mathcal{K} is Hermitian *i.e.* $K(x, y) = \overline{K(y, x)}$ then \mathcal{K} is a normal operator; see [21, p.27]. This may be used as an important sufficient condition. For the case where S is a sphere, we can prove the following result concerning the continuous problem.

THEOREM 4.5

If an operator \mathcal{K} is a combination of the identity operator \mathcal{I} and potential operators L_k, M_k, M_k^T and N_k or their products, then it is normal.

Proof. Following [3], when S is a sphere, all operators forming \mathcal{K} have the orthogonal spherical harmonics $S_n^m(\cdot)$ as their eigenfunctions and hence so will \mathcal{K} , implying that \mathcal{K} is normal; see [75]. □

Remarks

- (a). In view of Theorem 4.5 and the preceding remarks, we can expect the eigenvalues of AA^* to cluster around some fixed point in a similar manner to that of A . This accumulation point is just the square of that for A .
- (b). Much work has been done in the field of CG methods with preconditioners; (refer to [16, Ch.8] and [46, Ch.10] and the references therein). In theory, preconditioning is very attractive since it can reduce the condition number and hence improve the speed of convergence. However no such precondi-

tioners exist even for the case of solving integral equations with compact operators, which can preserve the eigenvalue clustering pattern as well as reduce the condition number.

4.4 Numerical results and comparison

Here we consider the solution of the exterior acoustic problem in both 2 and 3 dimensional space. The domain of integration S is chosen to be a family of ellipses in 2D, characterised by the equation $(x/a)^2 + (y/b)^2 = 1$ and axisymmetric ellipsoids in 3D, characterised by $(x/a)^2 + (y/a)^2 + (z/c)^2 = 1$. We do not discuss the details of the underlying discretization method, as it should not greatly affect the efficiency or otherwise of the conjugate gradient method, provided the resulting linear systems mimic the spectral properties of the continuous equations. Numerical methods presented here are based on the point collocation method (refer to the panel method of §2.1), where the unknown function is approximated by a constant over each element. Throughout the section, the **ALGORITHM – Conjugate Gradients** presented in last section is used with the initial guess $\underline{x}^{(0)} = [0, 0, \dots, 0]^T$.

Dirichlet Problem

Here we consider the 2-dimensional problem (§3.5.2). In Figs.4.1-4.2, we plot the approximate eigenvalue spectra with compact operators for a typical case of $a = 0.5$ and $b = 1.5$. We have computed the eigenvalues in four discrete cases with $N = 50, 100, 200$ and 300 collocation points respectively. We note that as expected the eigenvalues cluster around 1 and the number of very distinct eigenvalues remains almost the same as N increases. The results from our nu-

merical calculations are summarised in Tables 4.1-4.2, for various choices of the problem and method parameters. The surface parameters a and b are chosen so that $d = (a + b)/2$, the typical length of the domain, is unity. In Tables 4.1-4.2, μ is the actual number of steps of the CG method required in order for the root mean square (RMS) norm of the residual for the approximate solution defined by $\left[\sum_1^N r_i^2 / N \right]^{1/2}$ to be less than the required tolerance τ (where r_i is the residual of the i -th equation). Furthermore, C is the 2-norm condition number of $A.A^*$, N is the size of the matrix, k is the wavenumber and η is the coupling parameter. The actual problem we are solving is equivalent to that of having one point source with strength $(2+3i)$ placed at point $(0.0,0.5)$; refer to §3.5.2. A blank entry in tables 4.1-4.3 indicates that the value of its corresponding parameter has not been changed from its previous value. In the Table 4.1, we compare CPU times on PRIME 850 for the CG method with $\tau = 10^{-6}$ to those of direct solution.

From the Table 4.1, we note that the CG method reduces the CPU times by substantial amounts. But in comparison to Tables 3.4-3.5, it is not as efficient as the multigrid type methods. From the Table 4.2, we can draw the following two conclusions :

- (a). Increasing N does not in general change the essential properties of the matrices approximating the underlying integral operator and hence for a given tolerance leaves μ , the required number of CG steps, unchanged. In general, μ is quite small and also decreasing τ does not increase μ substantially.
- (b). The choice of the coupling parameter $\eta(k) = ik/2$ (see §2.3) is useful in improving the condition number of the continuous operator and hence that of the matrix approximating it. It does not however necessarily reduce μ

as varying η changes the eigenvalues and affects their distributions slightly.

Neumann Problem

Here we consider the 3-dimensional problem (refer [3] and [10]). On discretizing the non-regularised equation (refer Theorem 2.12), involving the non-compact operator N_k , there is usually no clustering of the eigenvalues of A and indeed the eigenvalues and the condition number become larger in modulus as N is increased; see (4.25). In this case, a direct linear solver or a multigrid type method should be used; refer to [6] for some initial results. Theoretically preconditioned CG methods are potentially attractive methods for solving such linear systems arising from discretization of integral equations with non-compact operators — unfortunately at present such general preconditioners are not available.

Below we adopt the regularised formulation (1.59) and present the numerical results in table 4.3. The parameters and also the conclusions are much the same as those for the Dirichlet problem. Here $[\alpha, \beta]$ and m are as in Theorem 4.2 (for the matrix AA^*) and $\ell = 0$ in all cases. The surface parameters are chosen such that $d = (a + a + c)/3 = 1$. Furthermore, the actual problem being solved here is equivalent to that of having one point source with strength $(2+3i)$ placed at point $(0.0, 0.0, 0.2)$; refer to [10].

We point out here that due to the limitations on the available dynamic memory on our computer we were unable to run the 3D problem for larger values of N . Nevertheless the results in table 4.3 clearly demonstrate, among other things, the dense clustering pattern of the eigenvalues and also the effect of the choice of the coupling parameter as $\eta(k) = ki$ in reducing the condition number of the matrix as well as μ (slightly). We observe that relatively few CG steps are required to

Table 4.1: Direct method and CG method for Dirichlet problem (CPU times)

| N | Set up | Direct | Conjugate gradients | | |
|-----|--------|--------|---------------------|-------------------|-------------------|
| | | | $b/a = 1$ | $b/a = 3$ | $b/a = 4$ |
| 81 | 59.1 | 15.3 | 11.3 ($\mu=5$) | 17.5 ($\mu=9$) | 17.5 ($\mu=9$) |
| 243 | 527.5 | 400.1 | 87.3 ($\mu=5$) | 159.8 ($\mu=9$) | 159.8 ($\mu=9$) |

yield a sufficiently accurate approximation \underline{x}_N to \underline{x}^* .

Fig.4.1 Approximate Eigenvalue Spetrum of $A = (I - K)$

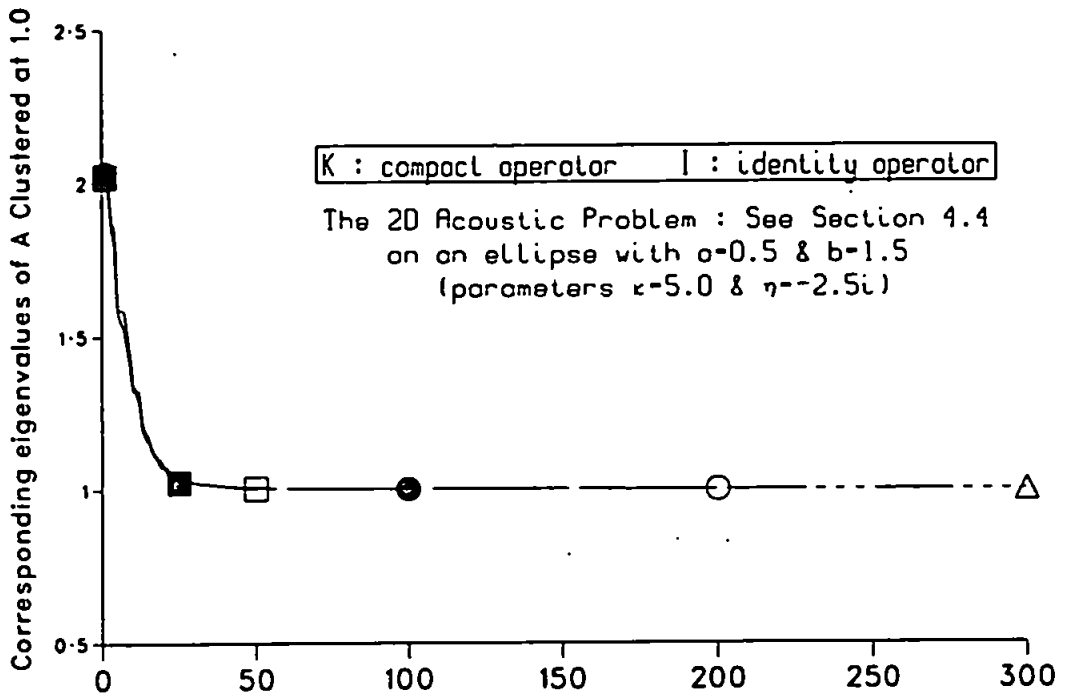


Fig.4.2 Approximate Eigenvalue Spetrum of $B = AA^*$

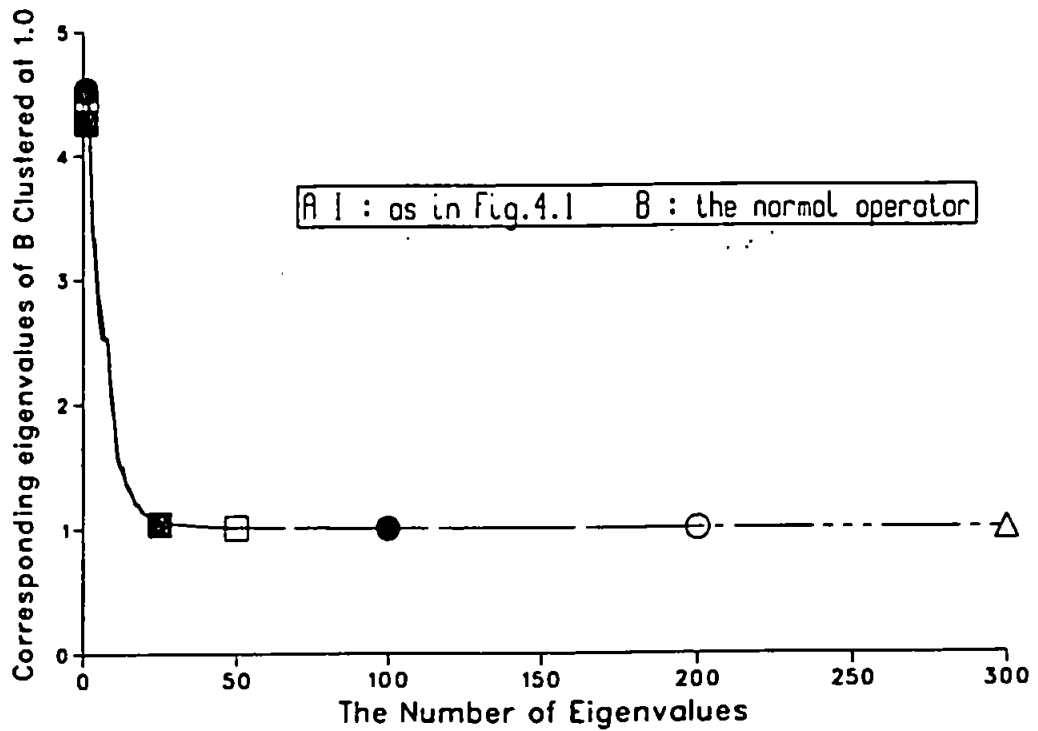


Table 4.2: CG method for Dirichlet problem in 2D

| a | b | k | η | N | C | τ | μ |
|-----|------|------|--------|-----|------|-----------|-------|
| 1.0 | 1.0 | 5.0 | i | 100 | 9.8 | 10^{-4} | 6 |
| | | | | 200 | 9.8 | 10^{-4} | 6 |
| | | | | 300 | 10.0 | 10^{-4} | 6 |
| | | | | 300 | 10.0 | 10^{-6} | 9 |
| 1/2 | 3/2 | 5.0 | i | 300 | 7.3 | 10^{-6} | 9 |
| | | | | 300 | 7.3 | 10^{-6} | 9 |
| | | | 2.5i | 100 | 16.2 | 10^{-4} | 9 |
| | | | | 300 | 16.2 | 10^{-6} | 12 |
| 1/3 | -1/3 | 5.0 | 2.5i | 300 | 11.3 | 10^{-6} | 16 |
| | | | | 200 | 13.8 | 10^{-6} | 14 |
| | | | | 200 | 19.2 | 10^{-6} | 17 |
| | | 10.0 | 5.0i | | | | |

Table 4.3: CG method for Neumann problem in 3D

| a | c | k | η | N | C | (α, β) | m | τ | μ | |
|-----|-----|-----|--------|------|------|-------------------|--------------|-----------|-----------|----|
| 1.0 | 1.0 | 5.0 | i | 50 | 32.5 | (0.19, 1.16) | 4 | 10^{-4} | 15 | |
| | | | | 100 | 34.7 | | 4 | 10^{-4} | 16 | |
| | | | 2.0 | 2.0i | 100 | 8.0 | (0.27, 0.38) | 2 | 10^{-4} | 12 |
| | | | | | 100 | 8.0 | | 4 | 10^{-4} | 9 |
| 3/4 | 3/2 | 2.0 | i | 50 | 14.2 | (0.26, 0.44) | 6 | 10^{-4} | 14 | |
| | | | | 2.0i | 50 | | 7.2 | 5 | 10^{-4} | 11 |
| | | | | | 100 | | 7.3 | 5 | 10^{-4} | 12 |
| 1/2 | 2 | 2.0 | 2.0i | 50 | 6.4 | (0.26, 0.59) | 4 | 10^{-4} | 11 | |
| | | | | 100 | 6.4 | | 4 | 10^{-4} | 12 | |

Chapter 5

Numerical Solution of Boundary Element Equations on Non-smooth Boundaries

In this Chapter, we study the problem of solving boundary integral equations (BIE) defined on non-smooth boundaries. Here in general the resulting integral operator is no longer compact, though bounded, and the solution is non-smooth. In particular, we investigate the boundary integral equations arising from reformulation of a 2D Helmholtz equation with the Dirichlet boundary condition. Using Mellin transforms and the theory of singular integral equations (SIE) in §5.1, we first obtain the explicit form of singular solutions due to the boundary non-smoothness. Then in §5.2, both the collocation and the iterated collocation methods are applied to solve the integral equation with a non-compact operator. The singularity in the solution causes the slow convergence of existing methods without modifications. To restore the appropriate order of convergence, we adopt

the "mesh grading" technique in our numerical methods. The associated problem of numerical instability is discussed and the stability of discrete integral operator equations is established. We also give a brief discussion of other relevant numerical techniques. In §5.3, a numerical example is presented to illustrate and support the theoretical analysis of §5.2.

5.1 Singular behaviour of integral solutions

5.1.1 Introduction

By assuming that the integral boundary S is sufficiently smooth, we may establish the smoothness and the compactness of all relevant integral operators from reformulating the Helmholtz equation. Refer to [69]. These two properties of integral operators have been explicitly used throughout Chapters 2–4 when integral operator equations are solved by numerical methods. There, both the smoothness and the compactness are required in studying efficient numerical methods (see Chapter 2); while the latter is essential in developing iterative methods (see Chapters 3–4). However when the boundary of interest admits corners and edges (*i.e.* has geometric singularities), the solution to an integral operator equation will usually possess similar non-smooth behaviour near such singularities and the underlying integral operator is non-compact. Here we consider the solution of the Helmholtz equation on some non-smooth exterior domain in 2D.

As in §1.2 and §3.5.2, the 2D Helmholtz equation in a domain E exterior to some closed boundary S with the Dirichlet boundary condition is given by

$$\begin{cases} (\nabla^2 + k^2)\phi(p) = 0, & p \in E, \\ \phi(p) = f(p), & p \in S, \\ \lim_{r \rightarrow \infty} r^{1/2} \left\{ \frac{\partial \phi}{\partial r} - ik\phi(p) \right\} = 0, & p \in E, \end{cases} \quad (5.1)$$

The solution $\phi(p)$ of this equation may be represented by $\mathcal{H}_k\sigma$, where (see §1.4)

$$(\mathcal{H}_k\sigma)(p) = \int_S \left\{ \frac{\partial G_k}{\partial n_q} - \eta G_k \right\} \sigma(q) dS_q, \quad p \in E \quad (5.2)$$

where $\sigma(p)$ is an unknown density function. By imposing the Dirichlet boundary condition this yields the second kind integral equation (see §1.4)

$$\frac{\chi(p)}{2} \sigma(p) + \int_S \left\{ \frac{\partial G_k}{\partial n_q}(p, q) - \eta G_k(p, q) \right\} \sigma(q) dS_q = f(p), \quad p \in S \quad (5.3)$$

where $\chi(p)\pi$ is the internal angle at point p between the two tangents (note that $\chi(p) = 1$ at all smooth points). In (5.3), $G_k(p, q)$ is the fundamental solution for the Helmholtz equation and η is a non-zero coupling parameter required to ensure the uniqueness of $\sigma(p)$ for any k . Here we choose $\eta = ki/2$ as this choice can be shown to improve the conditioning of the equation (5.3). (See [3], [68] and §1.4).

On a non-smooth boundary S , the integral operator \mathcal{H}_k is no longer compact and the solution σ may not be smooth, even if f is. Refer to [18], [19], [49]. The solvability of an integral equation such as (5.3) on piecewise smooth boundaries may be established through the generalized Fredholm theory; (refer to the remark in §1.1 and [66]). As for the behaviour of the solution σ , the theory is not complete if the boundary S is non-smooth. In the case of Laplace's equation, analysis has been carried out to obtain the analytical properties of solutions for polygonal domains ([37],[42]). For the Helmholtz's equation, only the dipole distribution (the double layer potential) for the interior problem was heuristically analysed in

[82]. As is known (see §1.4), representation of solution by the dipole distribution does not guarantee the existence of an unique solution for the resulting boundary integral equation at all wavenumbers.

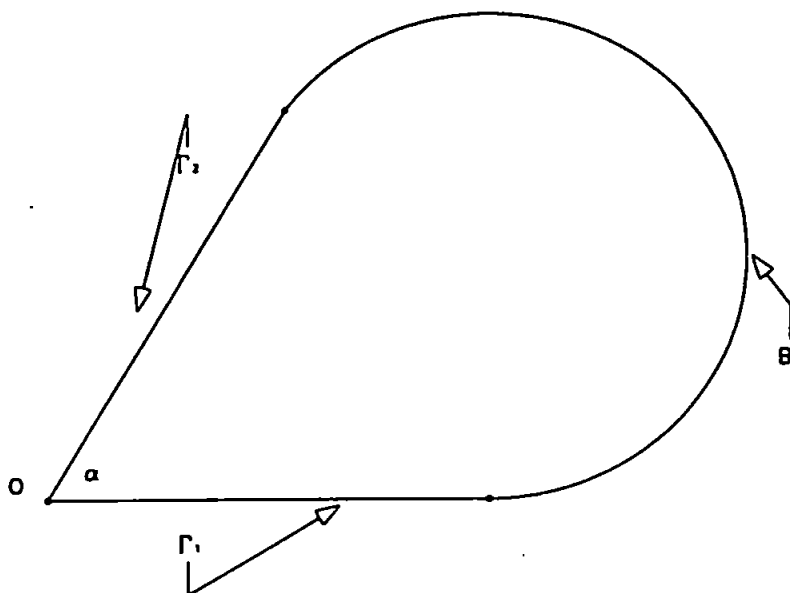
The precise knowledge of the solution behaviour is generally of fundamental importance. In practice, most of the commonly-used numerical techniques for solving integral equations are derived and analysed based on some global assumption of the behaviour of solutions. Often the solution to the integral equation is assumed to belong to the spaces of C^2 or C^4 functions (see [51]). Then the order of convergence of a particular numerical method can be determined accordingly using classical analysis. Here in this section, we analyse the theoretical behaviour of the solution of the boundary integral formulation for the exterior Helmholtz problem on polygonal domains by considering the formulation (5.3) which is valid for all wavenumbers.

Without essential loss of generality, let us suppose that the non-smooth boundary S has a single corner point at o and comprises of two straight lines Γ_1 and Γ_2 and a smooth curve B , as shown in *Fig.5.1*, where the angle between Γ_1 and Γ_2 is denoted by α and the point o is set to be the origin in Cartesian coordinates with Γ_1 along the x-axis. Let us further assume that the lengths of both Γ_1 and Γ_2 are ℓ and the closed boundary S is defined in the anticlockwise direction as depicted. In fact the curves may be denoted by

$$\begin{aligned} \Gamma_1 & : (s, 0), & 0 \leq s \leq \ell, \\ B & : (x(s), y(s)), & \ell < s < t_1, \\ \Gamma_2 & : ((T - s) \cos \alpha, (T - s) \sin \alpha), & t_1 \leq s \leq T, \end{aligned}$$

where s is the arc length measured anticlockwise from the corner point o and

Figure 5.1: 2D Boundary Curve S with a corner at point o



$T = l_1 + l_2$ is the total length of boundary S . Note that Γ_2 may also be denoted by

$$\Gamma_2 : (s \cos \alpha, s \sin \alpha), \quad 0 \leq s \leq l_2,$$

where s is the arc length measured clockwise from the corner point o . Recall from Chapter 1 that the fundamental solution in 2D is given by the Hankel function of the first kind

$$G_k(p, q) = \frac{i}{4} H_0^{(1)}(kr), \quad r = |p - q|, \quad (5.4)$$

where the derivative of $H_0^{(1)}(x)$ is

$$\frac{dH_0^{(1)}(x)}{dx} = -H_1^{(1)}(x). \quad (5.5)$$

In our study, we shall require the following expansions of the Hankel functions near $x = 0$ (see [97, Ch.3])

$$H_0^{(1)}(x) = \frac{2i}{\pi} \log x + R_0(x), \quad (5.6)$$

$$H_1^{(1)}(x) = -\frac{2i}{\pi x} + \frac{i}{\pi} x \log x + R_1(x), \quad (5.7)$$

where functions $R_0(x)$ and $R_1(x) = o(x^2) + xP(x^2)$ are analytical (differentiable), with $P(\cdot)$ denoting an absolutely convergent power series. Note that $\frac{d[R_1(x)/x]}{dx}$ is continuous in the vicinity of $x = 0$.

We are primarily interested in the behaviour of solution σ in the neighbourhood of o where $\sigma(p)$ may not be smooth. In what follows, we shall proceed our investigation in three subsections. In §5.1.2, we rewrite the boundary integral equation (5.3) defined on S into a sum of integrals using kernel expansions, each integral defined on one of the three segments of S . Then we shall form a new singular integral equation which contains the most singular integral. In §5.1.3, we apply the Mellin transform to the new singular integral equation to obtain an equation more amenable to classical analysis — the Cauchy type singular integral equation. Finally in §5.1.4, in order to determine the analyticity of the Mellin transform of σ near point o we shall use the theory of solutions of singular integral equations. We analyse such analyticity information by using the inverse Mellin transform to reveal the singular behaviour of solution σ . We leave the problem of numerical solution for (5.3) until §5.2.

5.1.2 Boundary integral equations

Consider the boundary integral equation (5.3). Using (5.6)–(5.7), it can be written as

$$\frac{\sigma(p)}{2} - \frac{i}{4} \int_S \{ \eta \mathbf{H}_0^{(1)}(kr) + k \mathbf{H}_1^{(1)}(kr) \text{Grad}(r) \cdot n_q \} \sigma(q) dS_q = f(p), \quad (5.8)$$

$$p \in S/\{0\}.$$

To study the behaviour of the solution of (5.8) near $p = o$, let us write it more explicitly for the cases where $p \in \Gamma_1$ and $p \in \Gamma_2$. We have for $p \in \Gamma_1$:

$$\begin{aligned}
\frac{\sigma(p)}{2} &= \frac{i\eta}{4} \int_0^\ell \mathbf{H}_0^{(1)}(k|s-s'|)\sigma(s',0)ds' \\
&- \frac{s \sin \alpha}{2\pi} \int_0^\ell \frac{\sigma(p')ds'}{r_{s'}^2} \\
&+ \frac{k^2 s \sin \alpha}{4\pi} \int_0^\ell \log(kr_{s'})\sigma(p')ds' \\
&- \frac{i}{4} \int_0^\ell \left\{ \eta \mathbf{H}_0^{(1)}(kr_{s'}) + \frac{ksR_1(kr_{s'}) \sin \alpha}{r_{s'}} \right\} \sigma(p')ds' \quad (5.9) \\
&- \frac{i}{4} \int_B \left\{ \eta \mathbf{H}_0^{(1)}(kr_s) + k\mathbf{H}_1^{(1)}(kr_s) \text{Grad}(r_s) \cdot n_q \right\} \sigma(q)dS_q \\
&= f(p), \quad 0 < s \leq \ell,
\end{aligned}$$

where $q = (x(t), y(t)) \in B$, $r_s = |p - q|$ and $p' = (s' \cos \alpha, s' \sin \alpha) \in \Gamma_2$ with $r_{s'} = |p - p'|$. Also for $p = (s \cos \alpha, s \sin \alpha) \in \Gamma_2$, we have similarly

$$\begin{aligned}
\frac{\sigma(p)}{2} &= \frac{i\eta}{4} \int_0^\ell \mathbf{H}_0^{(1)}(k|s-s'|)\sigma(p')ds' \\
&- \frac{s \sin \alpha}{2\pi} \int_0^\ell \frac{\sigma(s',0)ds'}{r_{s'}^2} \\
&+ \frac{k^2 s \sin \alpha}{4\pi} \int_0^\ell \log(kr_{s'})\sigma(s',0)ds' \\
&- \frac{i}{4} \int_0^\ell \left\{ \eta \mathbf{H}_0^{(1)}(kr_{s'}) + \frac{ksR_1(kr_{s'}) \sin \alpha}{r_{s'}} \right\} \sigma(s',0)ds' \quad (5.10) \\
&- \frac{i}{4} \int_B \left\{ \eta \mathbf{H}_0^{(1)}(kr_s) + k\mathbf{H}_1^{(1)}(kr_s) \text{Grad}(r_s) \cdot n_q \right\} \sigma(q)dS_q \\
&= f(p), \quad 0 < s \leq \ell,
\end{aligned}$$

where again $q = (x(t), y(t)) \in B$, $r_s = |p - q|$ and $p' = (s' \cos \alpha, s' \sin \alpha) \in \Gamma_2$ with $r_{s'} = |p - p'|$. Here the case for $p \in B$ need not to be written down as it would be similar to equation (5.8).

In the remaining of this section, we shall denote by C^0 the space of complex and continuous functions in $[0, \infty)$ and by C^1 the space of complex and continuously differentiable functions in $[0, \infty)$, unless we specify otherwise. In order to

determine the smoothness of above integrals as functions of s (except those with the kernel $\frac{1}{s'^2 + s^2 - 2s's \cos \alpha}$), let us make the minimal assumption that $\sigma \in C^0$.

Then we can show that those integrals in (5.9) and (5.10) involving the boundary B or the kernel function R_1 define C^1 functions because the integrands are sufficiently smooth. The kernel of other integrals may be typified by

$$H_0^{(1)}(k\sqrt{s'^2 + s^2 - 2s's \cos \alpha'}) \quad (5.11)$$

where the angle α' may take any value (in particular $\alpha' \in [0, 2\pi)$). From relation (5.6), the logarithmic kernel is implicitly represented by (5.11) when $\alpha' = 0$. Then the continuity of such integrals follows immediately from the lemma below.

LEMMA 5.1

The single layer potential operator $L_k : C^0[0, \ell] \rightarrow C^0[0, \ell]$ defined by

$$L_k u(s) = \int_0^\ell H_0^{(1)}(k\sqrt{s'^2 + s^2 - 2s's \cos \alpha'}) u(s') ds' \quad (5.12)$$

is compact for any value of α' .

Proof. From expansion of (5.6) we can see the relation $H_0^{(1)}(kr) = A(s, s')B(s, s')$, with $A = |s - s'|^\gamma H_0^{(1)}(kr)$ bounded and $B = \frac{1}{|s - s'|^\gamma}$ ($0 < \gamma < 1$) weakly singular, satisfying the sufficient conditions for compact operators ([14, Ch.1]). Thus the lemma is proved. □

We have assumed that the solution σ is a C^0 function but not a C^1 function. Hence C^1 functions are considered to be sufficiently smooth not to contribute to the singular behaviour of σ . From the assumption $u \in C^0$, we cannot show that $L_k u$ defined by (5.12) has any additional smoothness. However $L_k u$ may possess some additional smoothness if we take u from some subspace of C^0 . Now let us

define a subspace of C^0 by

$$\bar{C}^0 = \{u : u \in C^0[0, \infty) \text{ and } u(s)/s^\rho \text{ is bounded for some } \rho > 0\}.$$

Later on we shall prove that in general the solution to (5.8) belongs to the space of \bar{C}^0 for some value of ρ that depends on the wedge angle α . Here using the space \bar{C}^0 , we have the following results.

THEOREM 5.2

If $u \in \bar{C}^0$, then $(L_k u)(s)$ defined by (5.12) with $\alpha' > 0$ is a C^1 function.

Proof. Write the derivative $\frac{dL_k u(s)}{ds}$ as $D(s) = k \int_0^t H_1^{(1)}(kr) \frac{s' \cos \alpha' - s}{r} u(s') ds'$ where $r = \sqrt{s'^2 + s^2 - 2s's \cos \alpha'}$. For any $s' > 0$, we have

$$\min_{s' \in [0, t]} r = \begin{cases} s' \sin \alpha', & \sin \alpha' \neq 0, \\ s', & \sin \alpha' = 0, \end{cases}$$

and $\left| \frac{s' \cos \alpha' - s}{r} \right| \leq 1$. Since $r H_1^{(1)}(kr)$ is bounded, we therefore have

$$\begin{aligned} \left| H_1^{(1)}(kr) \frac{s' \cos \alpha' - s}{r} u(s') \right| &\leq c_1 \left| \frac{u(s')}{s'^\rho} \right| \cdot \left| \frac{1}{s'^{1-\rho}} \right| \\ &\leq c_2 \left| \frac{1}{s'^{1-\rho}} \right|, \end{aligned}$$

where c_1, c_2 are constants independent of s, s' . Hence $L_k u \in C^1$. □

THEOREM 5.3

If $u \in \bar{C}^0$, then $(L_k u)(s)$ defined by (5.12) with $\alpha' = 0$ is a C^1 function.

Proof. Define a function $E(s) = \int_0^t \log |s - t| u(t) dt$. Then we have $(L_k u)(s) = \frac{2i}{\pi} E(s) + v(s)$, where $v(s)$ is a C^1 function (using (5.6)). Obviously $E(0)$ exists.

For $s > 0$, we use the series expansion :

$$\log |s - t| = \begin{cases} \log s - \sum_{j=1}^{\infty} \frac{1}{j} s^{-j} t^j, & 0 \leq t < s, \\ \log t - \sum_{j=1}^{\infty} \frac{1}{j} s^j t^{-j}, & s < t \leq \ell, \end{cases}$$

to obtain

$$\begin{aligned}
 E(s) &= \int_0^s \log |s-t| u(t) dt + \int_s^\ell \log |s-t| u(t) dt \\
 &= \log s \int_0^s u(t) dt - \sum_{j=1}^{\infty} \frac{1}{j s^j} \int_0^s t^j u(t) dt \\
 &\quad + \int_s^\ell \log t u(t) dt - \sum_{j=1}^{\infty} \frac{s^j}{j} \int_s^\ell t^{-j} u(t) dt.
 \end{aligned}$$

Therefore $L_k u \in C^1$. □

Thus we can conclude that all integrals in (5.9) and (5.10) except those with the kernel $\frac{1}{s'^2 + s^2 - 2s's \cos \alpha}$ define not only C^0 functions of s but also C^1 functions if we assume $\sigma \in \bar{C}^0$. As we are interested in the behaviour of $\sigma(p)$ near $p = o$ i.e. $s = 0$, let us introduce the notation

$$\sigma_1(s) = \sigma(s, 0), \quad \sigma_2(s) = \sigma(s \cos \alpha, s \sin \alpha),$$

$$\bar{f}_1(s) = f(s, 0), \quad \bar{f}_2(s) = f(s \cos \alpha, s \sin \alpha),$$

and

$$\psi_1 = \sigma_1 + \sigma_2, \quad \psi_2 = \sigma_1 - \sigma_2,$$

$$f_1 = \bar{f}_1 + \bar{f}_2, \quad f_2 = \bar{f}_1 - \bar{f}_2, \quad 0 \leq s \leq \ell.$$

Then using the above equations and by forming (5.9) \pm (5.10), we may transform (5.8) into the following uncoupled equations

$$\frac{\psi_j}{2} \mp \frac{s \sin \alpha}{2\pi} \int_0^\ell \frac{\psi_j(s') ds'}{s'^2 + s^2 - 2s's \cos \alpha} = F_j(s), \quad (5.13)$$

$$\text{for } j = 1, 2 \text{ and } 0 < s \leq \ell,$$

where $F_j(s)$ are continuous C^0 functions ($j = 1, 2$). Now we remark that F_j is originated from four parts (comparing with (5.8)) i.e.

$$F_j(s) = V_j(s) + (X_k \psi_j)(s) + (\bar{X}_k \sigma)(s) + (Y_k \psi_j)(s) \quad (5.14)$$

where $X_k, \bar{X}_k, Y_k : C^0 \rightarrow C^0$ are compact operators (in particular $C^0 \xrightarrow{X_k, \bar{X}_k} C^1$ and $\bar{C}^0 \xrightarrow{Y_k} C^1$) from Lemma 5.1 and Theorems 5.2-5.3 and $V_j(s)$ represents

some linear combination of the given function f . Clearly we have established that $F_j \in C^1$ if $\psi_j \in \bar{C}^0$ and $f \in C^1$, allowing us to concentrate on the singular part of the equation (5.13).

Remark :

In general if $\sigma(o) \neq 0$, the simple change of variable of $\tilde{\sigma}(p) = \sigma(p) - \sigma(o)$ can reset the integral equation (5.8) with the new unknown function $\tilde{\sigma}$. Further we have $\tilde{\sigma} \in \bar{C}^0$. Refer to [9] and [49] for further discussion.

5.1.3 Application of Mellin transforms

To study the singular integral equation (5.13), we first need to know more about its singularity type. To this end, we now employ the very useful analytical tool of Mellin Transforms to convert (5.13) into some better known forms of singular integral equations; (refer to [95], [22]). The generalised Mellin transform of a function $\psi(s)$ is defined by

$$\Delta(\xi) = \int_0^{\infty} \psi(s)s^{\xi-1} ds$$

with its inverse transform given by

$$\psi(s) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \Delta(\xi)s^{-\xi} d\xi,$$

where the constant $c \in (c_1, c_2)$ is a real number(to be specified). We note that the change of variable $s = e^{-x}$ will reveal the close relationship between the Mellin transform and the Fourier transform *i.e.*

$$\Delta(i\xi) = \int_{-\infty}^{\infty} e^{-i\xi x} \psi(e^{-x}) dx, \quad -\infty < \xi < \infty.$$

Applying the Mellin transform to both sides of (5.13), we immediately obtain the corresponding equations

$$\frac{\Delta_j(\xi)}{2} \mp \frac{\sin \alpha}{4\pi^2 i} \int_{c-i\infty}^{c+i\infty} d\xi' \Delta_j(\xi') \int_0^\infty s^\xi ds \int_0^\ell \frac{(s')^{-\xi'} ds'}{s'^2 + s^2 - 2s's \cos \alpha} = \Phi_j(\xi), \quad (5.15)$$

for $j = 1, 2$ and $c - i\infty < \xi < c + i\infty$.

Due to the fact that (5.13) is only required for a finite interval, the existence of Mellin transforms of $\psi_j(s)$ and $F_j(s)$ can be ensured by continuing the functions. For a locally integrable function on $(0, \infty)$ the definition of Mellin transform may be generalised (see [22]). In the domain $c_1 < \text{Re}(\xi) < c_2$ where Mellin transforms exist, both $\Delta_j(s)$ and $\Phi_j(s)$ are analytical since $s^{\xi-1}$ is an entire function with respect to ξ (see [100, p.92]). Now using the equality $s'^2 + s^2 - 2s's \cos \alpha = (s' - se^{i\alpha})(s' - se^{-i\alpha})$, we can carry out the integration ([47, p.284])

$$\int_0^\ell \frac{(s')^{-\xi'} ds'}{s'^2 + s^2 - 2s's \cos \alpha} = \frac{\ell^{(1-\xi')}}{2is^2(1-\xi') \sin \alpha} \left[e^{i\alpha} \mathbf{F}_1^2(1, \xi'; 1 + \xi'; \frac{\ell}{se^{-i\alpha}}) - e^{-i\alpha} \mathbf{F}_1^2(1, \xi'; 1 + \xi'; \frac{\ell}{se^{i\alpha}}) \right], \quad (5.16)$$

where $0 < s < \ell$ and the hypergeometric function is defined as usual by

$$\mathbf{F}_1^2(a, b; c; x) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{x^n}{n!}, \quad |x| < 1,$$

with the coefficients $(d)_n = (d)(d+1)(d+2)\cdots(d+n-1)$ and $(d)_0 = 1$. Since the modulus $|\frac{\ell}{se^{\pm i\alpha}}|$ may be larger than 1, we then require the Kummer's relations to transform (5.16) into hypergeometric functions of convergent series; (see [70, Ch.3]). This leads us to

$$\int_0^\ell \frac{(s')^{-\xi'} ds'}{s'^2 + s^2 - 2s's \cos \alpha} = \frac{\pi \sin(\pi - \alpha) \xi'}{2is \xi' \sin \alpha} \left[\mathbf{F}_1^2(1, \xi'; 1 + \xi'; \frac{se^{-i\alpha}}{\ell}) - \mathbf{F}_1^2(1, \xi'; 1 + \xi'; \frac{se^{i\alpha}}{\ell}) \right], \quad (5.17)$$

where we have used the equalities

$$\frac{\Gamma(2 - \xi')\Gamma(-\xi')}{\Gamma(1 - \xi')^2} = \frac{\xi' - 1}{\xi'} \quad \text{and} \quad \frac{\Gamma(2 - \xi')\Gamma(\xi')}{\Gamma(1)^2} = \frac{1 - \xi'}{\sin \pi \xi'}$$

Applying the series expansions (of F_1^2) to both (5.16) and (5.17), we may then obtain the function

$$W(\xi', s) \equiv \int_0^\ell \frac{(s')^{-\xi'} ds'}{s'^2 + s^2 - 2s's \cos \alpha} = \begin{cases} \sum_{n=1}^{\infty} \left(\frac{\ell}{s}\right)^n \frac{\sin n\alpha}{s(n - \xi')\ell^{\xi'} \sin \alpha}, & s > \ell, \\ \frac{\pi \sin(\pi - \alpha)\xi'}{s^{\xi'+1} \sin \alpha \sin \pi \xi'} - \frac{1}{s\ell^{\xi'} \sin \alpha} \sum_{n=1}^{\infty} \left(\frac{s}{\ell}\right)^n \frac{\sin n\alpha}{n + \xi'}, & s < \ell, \end{cases} \quad (5.18)$$

where $W(\xi', s)$ at $s = 0$ or ℓ will not be required. Next we evaluate the following integral (relating to the Mellin transform)

$$\int_0^\infty s^\xi W(\xi', s) ds = \frac{\pi \ell^{\xi - \xi'} \sin(\pi - \alpha)\xi'}{(\xi - \xi') \sin \alpha \sin \pi \xi'} + \frac{\ell^{\xi - \xi'}}{\sin \alpha} \sum_{n=1}^{\infty} \left[\frac{\sin n\alpha}{(n - \xi')(n - \xi)} - \frac{\sin n\alpha}{(n + \xi')(n + \xi)} \right], \quad (5.19)$$

where we assume that $Re(\xi) > Re(\xi')$, although both terms (for ξ, ξ') would have poles at integer points. But this can be cured if we choose c in the inverse Mellin transform such that $|c| < 1$ (so (5.19) is always valid). At this point, if we denote

$$r(\xi') = \frac{\sin(\pi - \alpha)\xi'}{\sin \pi \xi'}$$

and

$$R_j(\xi) = \Phi_j(\xi) \mp \frac{\ell^\xi}{4\pi^2 i} \sum_{n=1}^{\infty} \int_{c-i\infty}^{c+i\infty} \Delta_j(\xi') \left[\frac{\ell^{-\xi'}}{(n - \xi')(n - \xi)} - \frac{\ell^{-\xi'}}{(n + \xi')(n + \xi)} \right] d\xi',$$

with the understanding that the analyticity of R_j 's ($j = 1, 2$) are only determined by Φ_j 's (since the second term will be analytical everywhere except at the integer points), we then can obtain the following integral equation of Cauchy type

$$\frac{\Delta_j(\xi)}{2} \mp \frac{1}{4\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\ell^{\xi - \xi'} r(\xi') \Delta_j(\xi')}{\xi - \xi'} d\xi' = R_j(\xi), \quad (5.20)$$

for $j = 1, 2$, $c < \operatorname{Re}(\xi) < c_2$ and $|c| < 1$. Note that the right hand side of (5.20) also involves the unknown function $\Delta_j(\xi)$ (refer to (5.14)). This point will be discussed later in detail. In summary, we have established that (5.13) is essentially a Cauchy type singular integral equation; (see (5.20)). To solve the above equation (5.20), we shall use the Carleman-Vekua method; (refer to [44] and [79]).

5.1.4 Singular form of solutions of integral equations

Consider a new unknown function $S(\xi)$ determined by the Cauchy type integral

$$S_j(\tilde{\xi}) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{r(\xi') \ell^{\xi-\xi'} \Delta_j(\xi')}{\xi' - \tilde{\xi}} d\xi', \quad \forall \operatorname{Re}(\tilde{\xi}) \neq c. \quad (5.21)$$

Then using the Plemelj theorem (see [79, Ch.XV]) for boundary points $\operatorname{Re}(\xi) = c$, we have

$$\begin{aligned} S_j^+(\xi) &= \frac{1}{2} r(\xi) \Delta_j(\xi) + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{r(\xi') \ell^{\xi-\xi'} \Delta_j(\xi')}{\xi' - \xi} d\xi', \\ S_j^-(\xi) &= -\frac{1}{2} r(\xi) \Delta_j(\xi) + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{r(\xi') \ell^{\xi-\xi'} \Delta_j(\xi')}{\xi' - \xi} d\xi', \end{aligned}$$

where $S_j^+(\xi)$ and $S_j^-(\xi)$ are the two limits of $S_j(\tilde{\xi})$ taken from the right and left side of $\operatorname{Re}(\xi) = c$ respectively, with

$$S_j^+(\xi) - S_j^-(\xi) = r(\xi) \Delta_j(\xi), \quad (5.22)$$

and $S_j(\tilde{\xi})$ is analytical in $\{\tilde{\xi} : \operatorname{Re}(\tilde{\xi}) \in (c_1, c_2) / \{c\}\}$. With this notation, equation (5.20) can be replaced by the boundary integral problem

$$\Delta_j(\xi) \pm S_j^\pm(\xi) = 2R_j(\xi), \quad (5.23)$$

or the non-homogeneous Hilbert problem (using (5.22))

$$(1 \pm r(\xi)) S_j^\pm(\xi) - S_j^\mp(\xi) = 2R_j(\xi) r(\xi). \quad (5.24)$$

Combining (5.22) and (5.24) gives rise to the required solution

$$\Delta_j(\xi) = \frac{\pm S_j^-(\xi) + 2R_j(\xi)}{1 \mp r(\xi)}, \quad (5.25)$$

where $S_j^-(\xi)$ has no poles on $Re(\xi) = c$ and $S_j^-(\xi)$ is analytical on the left of $Re(\xi) = c$ except for negative integer points and the choice of $c = 0$ appears to be appropriate (refer to [82]).

Recall that the Inverse Mellin Transform of $\Delta_j(\xi)$ is given by

$$\begin{aligned} \psi_j(s) &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \Delta_j(\xi) s^{-\xi} d\xi \\ &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\pm S_j^-(\xi) + 2R_j(\xi)}{1 \mp r(\xi)} s^{-\xi} d\xi, \end{aligned} \quad (5.26)$$

using (5.25). Closing the integration contour from the left, we can then use the well-known theory of residues to evaluate the definite integral in (5.26) by looking at all the poles of the integrand; see [100, Ch.VI]. Those poles which are close to zero will determine the singular form of functions ψ_j 's i.e. solution σ .

THEOREM 5.4

If the given function $f(p) \in C^1$, then in \bar{C}_0 space the solution $\sigma(p)$ of equation (5.8) near the corner behaves like

$$\sigma(p) = Ar^\beta + \sigma_0(p), \quad \text{with } \beta = \min\left\{\frac{\pi}{\alpha}, \frac{\pi}{2\pi - \alpha}\right\}$$

where A is a constant, r is the distance of p from the corner and $\sigma_0(p)$ is a smoother function than r^β ($0 < \beta < 1$).

Proof. First, from (5.25), we know that apart from the possible integer poles¹ and those from the roots of

$$1 \mp r(\xi) = 0 \quad \text{i.e.} \quad \sin \pi \xi = \pm \sin(\pi - \alpha)\xi$$

¹An integer pole of $\xi = n$ for a function $\phi(x)$ corresponds to the non-singular component x^n of $\phi(x)$.

any other poles can only come from $\Phi_j(\xi)$, which is the Mellin transform of C^1 functions and whose poles ξ must satisfy that $Re(\xi) \leq -1$. As for the equation $1 \mp r(\xi) = 0$ above, its solutions (on the left half of $Re(\xi) = 0$) are given by

$$\begin{aligned} \xi &= -\frac{(2n-1)\pi}{2\pi-\alpha}, -\frac{2n\pi}{\alpha}, \text{ for } +; \\ \xi &= -\frac{(2n-1)\pi}{\alpha}, -\frac{2n\pi}{2\pi-\alpha}, \text{ for } -, \quad n = 1, 2, \dots \end{aligned}$$

Hence using the theory of residues completes the proof. \square

To carry out the convergence analysis of numerical methods in the next section, we now specify the necessary space setting. Following the above theorem, we can state that $\sigma \in \tilde{C}^0$ with the specific value of $\rho = \beta$ where β is given in Theorem 5.4. To make use of the numerical analysis results from the literature, we shall replace \tilde{C}^0 by another general subspace of C^0 . This is defined by

$$C_{\mu}^r = \{x : \|x(s) - x(0)\|_{r,\mu} < \infty\}$$

with the norm

$$\|y\|_{r,\mu} = \max_{0 \leq \nu \leq r} \sup_{0 < s \leq 1} |s^{\nu-\mu} D^{\nu} y(s)|,$$

where D is the 1D differentiation symbol as introduced in §1.1. Denote by \tilde{C}_{μ}^r the space of those C_{μ}^r functions which vanish at 0. Then we have $\sigma \in \tilde{C}_{\beta}^r$ with β from Theorem 5.4 and $r = 0$. Note that C_{β}^r is a subspace of C^0 , which contains functions of complex values, and is similar to space settings from the literature; *e.g.*, see [9], [33] and [74, Ch.4].

5.2 Numerical solution of singular boundary integral equations

In general for a singular boundary integral equation where the singularities are due to the non-smooth boundary, we can write the underlying non-compact operator as $\mathcal{G} + \mathcal{C}$ with \mathcal{G} a bounded linear operator and \mathcal{C} a compact operator. In particular, we may take \mathcal{G} to be the sum of wedge operators and \mathcal{C} is usually called the compact perturbation. The method for solving such an integral equation is first to study the so-called model integral equation with the operator \mathcal{G} alone and then to apply the results obtained to the original integral equation with the operator $\mathcal{G} + \mathcal{C}$.

In this section, we investigate the numerical solution of the boundary integral equation (5.13) from reformulation of the exterior Helmholtz equation defined on the non-smooth boundary S with a corner. Following the above general schema, we first form the model integral equation with the wedge operator in §5.2.1. Then we apply both collocation and iterated collocation methods (with non-uniform meshes) to the model equation in §5.2.2. The stability of the methods can only be established in special cases. To complete the theoretical analysis, we discuss in §5.2.3 the modified collocation and iterated collocation methods. We conclude the section in §5.2.4 with a brief discussion of other numerical methods.

5.2.1 The model integral equation

Let us now write the integral equation (5.13) in details as

$$\frac{\psi_j(s)}{2} \mp \frac{s \sin \alpha}{2\pi} \int_0^l \frac{\psi_j(s') ds'}{s'^2 + s^2 - 2s's \cos \alpha} + (Z_k \psi_j)(s) + (W_k \sigma)(s) = v_j(s),$$

for $j = 1, 2$ and $0 < s \leq \ell$, with $Z_k, W_k : C^0 \rightarrow C^0$ compact operators (refer to (5.14)). To simplify, it may be rewritten in an equivalent form

$$\begin{aligned} \psi_j(s) \mp (\mathcal{K}\psi_j)(s) + (\bar{Z}_k\psi_j)(s) + (W_k\sigma)(s) &= V_j(s), \\ 0 < s \leq \ell, \end{aligned} \tag{5.27}$$

where the operator \bar{Z}_k is still compact and $\mathcal{K} : C^0[0, 1] \rightarrow C^0[0, 1]$ is defined by

$$(\mathcal{K}\psi)(s) = \begin{cases} \frac{\pi-\alpha}{\pi} \psi(0), & s = 0, \\ \int_0^1 K\left(\frac{s}{t}\right) \psi(t) \frac{dt}{t}, & 0 < s \leq 1, \end{cases} \tag{5.28}$$

with its kernel

$$K(t) = \frac{\sin \alpha}{\pi} \frac{t}{1+t^2-2t \cos \alpha}. \tag{5.29}$$

The operator \mathcal{K} is the same as that arising from the solution of Laplace's equation; refer to [9], [33] and [74].

Without loss of generality let us consider the '-' sign case only and drop the subscript j for ψ and V . Note that in equation (5.27), both ψ and σ are unknowns. The complete equation for σ containing the operator \mathcal{K} may be written in the form of a system of operator equations; (refer to [74, Ch.5]). Since all other integral operators except \mathcal{K} are compact in C^0 , they can be considered to be the compact perturbations of the operator \mathcal{K} . So we shall concentrate on the reduced integral equation²

$$(I - \mathcal{K})u(s) = V(s), \quad 0 < s \leq 1, \tag{5.30}$$

which is referred to as the model integral equation. Throughout the remaining part of the chapter, we shall concentrate on the numerical analysis of (5.30). The

²Here the unknown ψ is replaced by u to avoid possible confusion later with the notation for basis functions ψ_j 's.

close relationship between (5.30) and the complete equation will be discussed towards the end of the next subsection.

For operator \mathcal{K} , the following results are known (see [74])

LEMMA 5.5

(i) In $C^0[0, 1]$, the spectrum of \mathcal{K} is given by

$$\text{spec}(\mathcal{K}) = \begin{cases} [0, \frac{\pi-\alpha}{\pi}], & 0 < \alpha < \pi, \\ [\frac{\pi-\alpha}{\pi}, 0], & \pi < \alpha < 2\pi. \end{cases}$$

(ii) If $0 < \alpha < 2\pi$, then

$$\|\mathcal{K} : C^0[0, 1] \rightarrow C^0[0, 1]\| = |\pi - \alpha|/\pi < 1,$$

$$\frac{\pi}{\pi + |\pi - \alpha|} \leq \|(\mathcal{I} - \mathcal{K})^{-1} : C^0[0, 1] \rightarrow C^0[0, 1]\| \leq \frac{\pi}{\pi - |\pi - \alpha|}.$$

(iii) $\mathcal{I} - \mathcal{K}$ is continuously invertible in \tilde{C}_g^r . □

The equation (5.30) can be shown to be strongly connected to a classical Wiener-Hopf equation (see [60, Ch.5]), the numerical analysis of which has been carried out in [9]; (see also [12]). In fact if in (5.30) we set $s = e^{-\theta}$, $t = e^{-\tau}$ and introduce the notation $\kappa(\theta) = K(e^{-\theta})$, $g(\theta) = V(e^{-\theta})$, and $v(\theta) = u(e^{-\theta})$, we obtain

$$v(\theta) - \int_0^\infty \kappa(\theta - \tau)v(\tau)d\tau = g(\theta), \quad \theta \in [0, \infty). \tag{5.31}$$

5.2.2 Collocation methods and their numerical analysis

We now consider the numerical solution of the model equation (5.30) by collocation and iterated collocation methods based on piecewise polynomials. Recall from §2.1 the definition of the space $S^{n,r}$ of piecewise polynomials based on a

mesh of $(n+1)$ points on $[a, b]$. Here we have $[a, b] = [0, 1]$. Therefore our mesh points are defined as

$$\Pi_n : 0 = \eta_0 < \eta_1 < \cdots < \eta_{n-1} < \eta_n = 1.$$

For $1 \leq i \leq n$ we set $I_i = (\eta_{i-1}, \eta_i]$, $h_{(i)} = \eta_i - \eta_{i-1}$ and $h_n = \max_{1 \leq j \leq n} h_{(j)}$. Then $S^{n,r}$ is the space of piecewise polynomials of order r on each subinterval I_i , $i = 1, \dots, n$; (see §2.1). To use the space $S^{n,r}$ for approximation of continuous functions, we can view it as the space spanned by the independent Lagrange polynomials $\{\psi_j\}_1^{N_n}$, where $N_n = nr$ is the dimension of space $S^{n,r}$ and ψ_j 's are discontinuous in $[0, 1]$; (refer to (2.12)). We shall use the space $S^{n,r}$ in this subsection, but in the next subsection, we shall need the slightly modified variants of $S^{n,r}$. For that purpose and along the similar lines of defining $S^{n,r}$, let us define $S_{u,v}^{n,r}$ to be the general space of piecewise polynomials of order r on each subinterval I_i , $i = u, \dots, v$ with $1 \leq u, v \leq n$ and $u < v$ (elements in $S_{u,v}^{n,r}$ are supposed to take zero value outside these subintervals). Obviously $S^{n,r} = S_{1,n}^{n,r}$ and $S^{n,r} = S_{1,u}^{n,r} \cup S_{u+1,n}^{n,r}$ for any $1 \leq u < n$.

As in §2.1, define the nodes of some quadrature rule on $[0, 1]$ by $\{\xi_j\}_1^r$ with $0 \leq \xi_1 < \cdots < \xi_r \leq 1$ and the collocation points on $[0, 1]$ by

$$s_j = \eta_{\nu-1} + \xi_l h_{(\nu)}, \quad 1 \leq j \leq N_n,$$

where $\nu = \text{INT}[(j-1)/r] + 1$, $l = j - (\nu-1)r$.

Then a projection operator $\mathcal{P}_n : C^0[0, 1] \rightarrow S^{n,r}$ is defined by

$$(\mathcal{P}_n \phi)(s) = \sum_{j=1}^{N_n} \phi(s_j) \psi_j(s), \quad s \in [0, 1], \quad (5.32)$$

which interpolates $\phi(s)$ at every collocation point, *i.e.*,

$$(\mathcal{P}_n \phi)(s_j) = \phi(s_j), \quad j = 1, \dots, N_n.$$

Using operator notation, the collocation approximation $u_n \in S^{n,r}$ to solution u of equation (5.30) is defined by (refer to §2.1)

$$(\mathcal{I} - \mathcal{P}_n \mathcal{K})u_n = \mathcal{P}_n V. \quad (5.33)$$

Further the product integration approximation u_n^* may be defined by

$$(\mathcal{I} - \mathcal{K} \mathcal{P}_n)u_n^* = V, \quad (5.34)$$

with the relation to u_n given by

$$u_n = \mathcal{P}_n u_n^* \quad (5.35)$$

and having the equivalent definition

$$u_n^* = V + \mathcal{K}u_n. \quad (5.36)$$

From equations (5.30) and (5.33), we can easily get (as in §2.1)

$$u - u_n = (\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1}(\mathcal{I} - \mathcal{P}_n)u \quad (5.37)$$

and then

$$\|u - u_n\| \leq \|(\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1}\| \cdot \|(\mathcal{I} - \mathcal{P}_n)u\|. \quad (5.38)$$

Here we are interested in the uniform or the supremum norm. From equations (5.30) and (5.34), we have similarly

$$u - u_n^* = (\mathcal{I} - \mathcal{K} \mathcal{P}_n)^{-1} \mathcal{K}(\mathcal{I} - \mathcal{P}_n)u \quad (5.39)$$

and further, using the identity

$$(\mathcal{I} - \mathcal{K} \mathcal{P}_n)^{-1} = \mathcal{I} + \mathcal{K}(\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1} \mathcal{P}_n, \quad (5.40)$$

we obtain for the product integration solution

$$\|u - u_n^*\| \leq [c_1 + c_2 \|(\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1}\|] \cdot \|\mathcal{K}(\mathcal{I} - \mathcal{P}_n)u\|, \quad (5.41)$$

where c_1, c_2 are generic constants independent of n and the solution u . Next to be considered are the following two questions :

(1). Does the stability hold *i.e.* , can we prove that³

$$\|(\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1}\| \leq c_3, \quad \forall n; \quad (5.42)$$

(2). Does the consistency hold for (5.39) and (5.41), *i.e.* , do the interpolation errors $\|(\mathcal{I} - \mathcal{P}_n)u\|$ and $\|\mathcal{K}(\mathcal{I} - \mathcal{P}_n)u\|$ converge to zero uniformly (and with a certain rate) as $n \rightarrow \infty$.

Let us first consider the second question. Due to the singular behaviour of u [using piecewise polynomial approximations on uniform meshes(see (2.15)) *i.e.*, $\eta_i = i/n$ ($i = 0, \dots, n$)], the convergence rate would be only $O(1/n^\beta)$. See [74, Ch.4], [81] and the numerical tests in §5.3. To restore the optimal order of convergence, we shall employ the so-called graded mesh(see (2.16))

$$\Pi_n : \eta_i = (i/n)^q, \quad i = 0, \dots, n, \quad q \geq 1. \quad (5.43)$$

Further the following convergence results may be proven (see [74, Ch.4]).

THEOREM 5.6

(i) *If the mesh grading exponent q in (5.43) satisfies $q \geq r/\beta$, then*

$$\|(\mathcal{I} - \mathcal{P}_n)u\|_\infty \leq c_4 n^{-r} \|u\|_{r,\beta};$$

(ii) *If ξ_1, \dots, ξ_r are chosen to be the Gauss-Legendre quadrature nodes shifted to $[0, 1]$ and $q \geq 2r/\beta$, then*

$$\|\mathcal{K}(\mathcal{I} - \mathcal{P}_n)u\|_\infty \leq c_5 n^{-2r} \|u\|_{2r,\beta},$$

³Recall from §2.1 that such a stability result holds if \mathcal{K} is compact.

where the constants c_4, c_5 only depend on q and r . □

We now turn to look at the first question, that of proving (5.42). This seems to be the difficult part of the analysis and the result is only proved in special cases. For piecewise constant approximations with $r = 1$ and $q \geq 1$ the proof is carried out in [74] and for the linear case with $r = 2$ it is only obtained in [18] for the uniform mesh ($q = 1$). In the case of $r = 2$ and $q > 1$, the proof of stability is known from [74, Ch.4] provided that $\pi/2 \leq \alpha \leq 3\pi/2$. Due to the lack of complete theoretical proof of the stability result (5.42) for collocation methods, we shall proceed to discuss their modified variants which overcome the problem.

At this point, we discuss the link between the numerical analysis of a compact perturbation equation of (5.30) and that of the model equation (5.30) using collocation methods. For simplicity of presentation, let us consider the following equation which is a compact perturbation equation of the model equation (5.30)

$$(I - \mathcal{K} - \mathcal{L})u = g, \quad g \in C^0[0, 1] \quad (5.44)$$

where \mathcal{L} is a compact operator in $C^0[0, 1]$. When using collocation methods for numerical solutions, all the above analysis for (5.30) will apply to (5.44) except that of the stability result. But the stability can also be established through the theorem below.

THEOREM 5.7

Let us consider equation (5.44) with \mathcal{K} as defined in (5.28) and let \mathcal{P}_n be the projection operator as in (5.32). If both $(I - \mathcal{K})^{-1}$ and $(I - \mathcal{K} - \mathcal{L})^{-1}$ exist in C^0 , then the stability result (5.42) for the model equation (5.30) ensures that for

the perturbation equation (5.44)

$$\|(\mathcal{I} - \mathcal{P}_n\mathcal{K} - \mathcal{P}_n\mathcal{L})^{-1}\| \leq c_6, \quad \text{for } n \text{ sufficiently large.}$$

Proof. From the following relation

$$(\mathcal{I} - \mathcal{P}_n(\mathcal{K} + \mathcal{L})) = (\mathcal{I} - \mathcal{P}_n\mathcal{K})(\mathcal{I} - (\mathcal{I} - \mathcal{P}_n\mathcal{K})^{-1}\mathcal{P}_n\mathcal{L}), \quad (5.45)$$

we shall try to show that $\|T_n^{-1}\| \leq c_7$ for sufficiently large n , where

$$T_n = \mathcal{I} - (\mathcal{I} - \mathcal{P}_n\mathcal{K})^{-1}\mathcal{P}_n\mathcal{L}.$$

Define $T = \mathcal{I} - (\mathcal{I} - \mathcal{K})^{-1}\mathcal{L}$. Then we see that T is invertible in C^0 since $T = (\mathcal{I} - \mathcal{K})^{-1}(\mathcal{I} - \mathcal{K} - \mathcal{L})$. Now from the proposition 1.4 of [11, p.3] (i.e. if T^{-1} exists and T_n converges to T uniformly, then T_n^{-1} is uniformly bounded), we only need to show that $\|T_n - T\| \rightarrow 0$ as $n \rightarrow \infty$. But we have

$$T_n - T = (\mathcal{I} - \mathcal{P}_n\mathcal{K})^{-1}(\mathcal{P}_n - \mathcal{I})(\mathcal{I} - \mathcal{K})^{-1}\mathcal{L}, \quad (5.46)$$

which converges to zero uniformly; (refer to Theorem 1.4). Hence the proof is complete. \square

As for the discussion of the relation of the complete equation (5.8) with the model equation (5.30), we refer the reader to [74, p.130]. The important point is that the model equation (5.30) mimics the essential singular features of the complete integral equation (5.8).

5.2.3 Modified collocation methods

The complete analysis of collocation projection methods has been recently carried out through making small modifications either by changes to interpolation on

intervals near geometric singularity [33] or by dropping one very small interval containing the singular part [9]. In both modified methods, the main modification is on the projection space of piecewise polynomials. We now introduce the two methods as applied to the model singular integral equation (5.30).

For the first modified method (Method I), we shall use the new space $S_i^{n,r}$ of piecewise polynomials instead of the space $S^{n,r}$ (as defined in the last subsection), where $S_i^{n,r} = S_{1,i}^{n,1} \cup S_{i+1,n}^{n,r}$. Here we employ the graded meshes Π_n 's as defined by (5.43). Then a projection operator $\bar{\mathcal{P}}_n : C^0[0, 1] + S_i^{n,r} \rightarrow S_i^{n,r}$ may be similarly defined by

$$(\bar{\mathcal{P}}_n u)(s) = \begin{cases} u(s_{i'-1/2}), & s \in I_{i'} \text{ and } i' \leq i, \\ \sum_{j=i'+1}^{N_n} u(s_j) \psi_j(s), & s \in I_{i+1} \cup \dots \cup I_n, \end{cases}$$

where ψ_j 's and s_j 's are the same as those defined in §5.2.2 using the graded mesh Π_n of (5.43) and $s_{i'-1/2} = (\eta_{i'-1} + \eta_{i'})/2$. The modified collocation solution $\bar{u}_n \in S_i^{n,r}$ may be defined by (refer to (5.33))

$$(\mathcal{I} - \bar{\mathcal{P}}_n \mathcal{K}) \bar{u}_n = \bar{\mathcal{P}}_n V, \quad (5.47)$$

and the modified product integration solution $\bar{u}_n^* \in C^0$ by (refer to (5.34))

$$(\mathcal{I} - \mathcal{K} \bar{\mathcal{P}}_n) \bar{u}_n^* = V, \quad (5.48)$$

or

$$\bar{u}_n^* = V + \mathcal{K} \bar{u}_n.$$

Then using Lemma 5.5(ii), i.e., the fact that $\|\mathcal{K}\| < 1$, we can show the following results of convergence and superconvergence; (see [33] for the proof).

THEOREM 5.8

(i) Suppose the mesh grading exponent q in (5.43) satisfies $q \geq r/\beta$. Then there exists an integer $i = i^*$ i.e. a space $S_{i^*}^{n,r}$ such that for all n sufficiently large

$$\|u - \tilde{u}_n\|_\infty \leq c_8 n^{-r} \|u\|_{r,\beta};$$

(ii) If ξ_1, \dots, ξ_r are chosen to be the Gauss-Legendre quadrature nodes shifted to $[0, 1]$ and $q \geq 2r/\beta$, then there exists an integer $i = i^*$ i.e. a space $S_{i^*}^{n,r}$ such that for all n sufficiently large

$$\|u - \tilde{u}_n^*\|_\infty \leq c_9 n^{-2r} \|u\|_{2r,\beta},$$

where the constants c_8, c_9 only depend on q and r . □

In our second modified method (Method II), we shall employ the following graded mesh in place of Π_n in (5.43)

$$\Pi_{n,\ell} : \eta_0 = 0, \quad \eta_i = \left(\frac{i+\ell}{n+\ell}\right)^q, \quad i = 1, \dots, n, \quad q \geq 1, \quad (5.49)$$

where $\ell \geq 0$ is some fixed integer. Note that for any $\ell \geq 0$, all $\Pi_{n-\ell,\ell}$ mesh points form a subset of $\Pi_{n,0}$ mesh points⁴. First we approximate (5.30) by the truncated equation

$$(\mathcal{I} - \mathcal{K}_\varepsilon)u_\varepsilon = V, \quad (5.50)$$

where

$$(\mathcal{K}_\varepsilon u)(s) = \int_{\varepsilon(n)}^1 K\left(\frac{s}{t}\right)u(t)\frac{dt}{t}, \quad s \in (0, 1],$$

with $\varepsilon(n) = \eta_1 = \left(\frac{1+\ell}{n+\ell}\right)^q \rightarrow 0$ as $n \rightarrow \infty$. To solve (5.50) by collocation methods, we here modify the space $S^{n,r}$ by using $\tilde{S}^{n,r} = S_{2,n}^{n,r}$. Then we may define the

⁴This fact will be used towards the end of the subsection.

projection operator $\tilde{\mathcal{P}}_n : C^0[0, 1] + \tilde{S}^{n,r} \rightarrow \tilde{S}^{n,r}$ by

$$(\tilde{\mathcal{P}}_n u)(s) = \begin{cases} 0, & s \in I_1, \\ \sum_{j=r+1}^{N_n} u(s_j) \psi_j(s), & s \in [0, 1] \setminus I_1, \end{cases}$$

where ψ_j 's and s_j 's are as defined as in §5.2.2 but using the mesh $\Pi_{n,\ell}$ of (5.49).

The projection solution is analogously given by (refer to (5.33))

$$(\mathcal{I} - \tilde{\mathcal{P}}_n \mathcal{K}_\epsilon) \tilde{u}_{\epsilon,n} = \tilde{\mathcal{P}}_n V, \quad (5.51)$$

and the modified projection solution $\tilde{u}_{\epsilon,n}^*$ by (refer to (5.34))

$$(\mathcal{I} - \mathcal{K}_\epsilon \tilde{\mathcal{P}}_n) \tilde{u}_n^* = V. \quad (5.52)$$

In such a setting, the following has been proved in [9].

THEOREM 5.9

(i) *If the mesh grading exponent q in (5.49) satisfies $q \geq r/\beta$, then for n sufficiently large*

$$\|u - \tilde{u}_n\|_\infty \leq O(n^{-r});$$

(ii) *If ξ_1, \dots, ξ_r are chosen to be the Gauss-Legendre quadrature nodes shifted to $[0, 1]$ and $q \geq 2r/\beta$ in (5.49), then for n sufficiently large*

$$\|u - \tilde{u}_n^*\|_\infty \leq O(n^{-2r}),$$

provided that ℓ is appropriately large in both cases. □

The two modified methods introduced above are both desirable and attractive theoretically. The reason is that we have the uniform boundedness of $(\mathcal{I} - \mathcal{P}_n \mathcal{K})^{-1}$.

But since they both involve one unknown parameter — i^* for the first method

(Method I) and ℓ for the second method (Method II), it may appear to hinder the implementation. In practice however, the choice of $i^* = 0$ for Method I and $\ell = 0$ for Method II is often satisfactory. Therefore it is possible and necessary to make full use of the theoretical results and to build a practical and reliable strategy in numerical implementation. The following two points will clarify the situation.

- (a). Often the possible ill conditioning of collocation equations (caused by the instability of discrete integral operator equations) can be revealed by the algorithm used for their numerical solutions, when starting with $i^* = 0$ for Method I or $\ell = 0$ for Method II. In this case, larger values of i^* or ℓ may be successively tried to restore the stability, which will be achieved and will not damage the asymptotic rate of convergence according to the theories.
- (b). Once the unmodified collocation coefficient matrix has been calculated and stored, it is not necessary to recalculate a new coefficient matrix when we switch to modified methods. Such a new matrix can be simply extracted and formed from its unmodified counterpart of size $N_n \times N_n$ with $N_n = nr$. In particular, by Method I, it will be of size $m \times m$ with $m = (n - i^*)r + i^*$ and, by Method II, of size $m \times m$ with $m = (n - \ell - 1)r$. The reduction in sizes effectively decreases the overall complexity in final solution.

5.2.4 Other numerical techniques

Although collocation methods discussed above are more often used in the engineering practice (see [24]), other numerical techniques such as Galerkin methods and Nyström methods may also be useful as is the case for solving a general second

kind integral equation (see [14] and Chapter 2). Extensions of these methods to problems defined on non-smooth boundaries have been recently established; see [32], [49] and the references therein. In [32], a complete error analysis of Galerkin methods for (5.30) using piecewise polynomials on graded meshes is shown without any modifications. As for Nyström methods, small modifications similar to those in Method I are required to prove uniform convergence on graded meshes; see [49] for further details.

5.3 Numerical experiments

We now present an example arising from the analysis of the boundary integral equation of the Helmholtz equation on a wedge in order to illustrate the effect of non-smooth solution on convergence rates. The equation to be solved can be represented in the form

$$\sigma(s) - \frac{i}{2} \int_0^1 \left\{ \eta \mathbf{H}_0^{(1)}(kr) + \frac{ks \sin \alpha}{r} \mathbf{H}_1^{(1)}(kr) \right\} \sigma(s') ds' = f(s),$$

$$0 < s \leq 1,$$

with $\alpha = \pi/10$, $k = 5.0$, $\eta = 2.5i$, $r = \sqrt{s'^2 + s^2 - 2s's \cos \alpha}$ and $f(s)$ is found accurately so the solution is $\sigma(s) = s^{1/2} e^{2\pi i} = s^{1/2}$.

We shall experiment with the product integration collocation method (§5.2.2–5.2.3) with piecewise constant and piecewise linear basis functions. Suppose that the interval $[0, 1]$ is subdivided into n small intervals with $0 = \eta_0 < \eta_1 < \dots < \eta_{n-1} < \eta_n = 1$. Then in the case of piecewise constants, we collocate at the mid-points of each interval, while in the case of piecewise linears we collocate at the two Gaussian points on each interval. The error is measured by (for a given

value of n with N_n collocation points)

$$E_n = \|\sigma_n - \sigma\| = \max\{\|\sigma_n^*(s_j) - \sigma(s_j)\|\}$$

over all collocated points s_j 's, where σ_n^* represents the product integration solution (refer to (5.34)). As in [63], using the error E_n , we may calculate the estimated order of convergence (EOC) by the formula $\text{EOC} = \log(E_n/E_{2n})/\log 2$. In Table 5.1 we show the results from using the uniform mesh *i.e.* using (5.43) with $q = 1$. Columns 3 and 6 denote the ratio between two errors of successive mesh sizes; while columns 4 and 7 list the corresponding EOC value. From the table, we see that all EOC values are below 0.5 but increasing as n increases. So we may expect the asymptotic rate of convergence to be $O(h^{1/2})$. Then we employ the graded mesh (5.43) with $q = 4$ for the piecewise constant case and with $q = 8$ for the piecewise linear case. The corresponding results are listed in Table 5.2. It can be envisaged that the new rates of convergence are $O(h^2)$ and $O(h^4)$ respectively, *i.e.* $\text{EOC} \approx 2$ and $\text{EOC} \approx 4$ respectively. It should be noted that here we need not apply the modified methods (§5.2.3) since no numerical instability was observed.

Table 5.1: Errors of the uniform mesh case

| N_n ($i^* = 0$) | Piecewise Constants | | | Piecewise Linears | | |
|------------------------|---------------------|---------------|-----|-------------------|---------------|-----|
| | E_n | $E_{n/2}/E_n$ | EOC | E_n | $E_{n/2}/E_n$ | EOC |
| 16 | .22E-1 | | | .12E-1 | | |
| 32 | .20E-1 | 1.11 | .15 | .11E-1 | 1.14 | .19 |
| 64 | .16E-1 | 1.19 | .25 | .88E-2 | 1.21 | .27 |
| 128 | .13E-1 | 1.25 | .32 | .69E-2 | 1.27 | .34 |

Table 5.2: Errors of the graded mesh case

| N_n ($i^* = 0$) | Piecewise Constants | | | Piecewise Linears | | |
|------------------------|---------------------|---------------|------|-------------------|---------------|------|
| | E_n | $E_{n/2}/E_n$ | EOC | E_n | $E_{n/2}/E_n$ | EOC |
| 16 | .73E-2 | | | .72E-2 | | |
| 32 | .25E-2 | 2.97 | 1.57 | .56E-3 | 12.8 | 3.68 |
| 64 | .72E-3 | 3.40 | 1.77 | .33E-4 | 17.1 | 4.09 |
| 128 | .19E-3 | 3.70 | 1.89 | .18E-5 | 18.1 | 4.18 |

Chapter 6

Iterative Solution of Boundary Element Equations on Non-smooth Boundaries

6.1 Introduction

In Chapters 3–4, we discussed the application of some iterative methods and established their convergence analysis for solving Fredholm integral equations of the second kind with compact operators. However as we have seen in the last chapter, boundary integral equations defined on non-smooth boundaries usually possess non-smooth operators. Therefore it is not a trivial task to extend or generalize the iterative techniques developed in Chapters 3–4 for numerical solutions of such integral equations. Obviously, the use of the conjugate gradient method as an efficient solver, as introduced in Chapter 4, does not appear to be feasible. The reason is that in general the spectra of the underlying integral operators are no

longer clustered (refer to Lemma 5.5). As for multigrid methods, some work has been carried out for the analysis and application of the methods; *e.g.* see [57], [86], [87] and [88]. The work so far on the convergence analysis of multigrid methods as applied to second kind integral equations with non-compact operators is incomplete in the sense that only uniform meshes have been considered, which are known to yield slowly converging approximations. Also the existing analysis is mostly centred on proving the convergence of multigrid methods but the equally important problem of overall efficiency is not fully studied. Furthermore, in all these papers, the stability of discrete operators is only assumed, though following the work of [18] such an assumption may be justified when employing uniform meshes. In this chapter we shall use the convergence results available from Chapter 5 so as to prove the convergence of multigrid methods for the solution of the discrete equations. Therefore our analysis also ensures the convergence of the discrete approximations to the solution of integral equations with optimal orders. We shall also report on our experiments with the conjugate gradient (CG) method as applied to some non-smooth integral equations.

As concluded in Chapters 3-4, for second kind integral equations with compact operators, the two grid methods are more efficient than the conjugate gradient method and they are almost as efficient as multigrid methods, yet being much easier to implement. Hence in this Chapter we shall confine ourselves to the study of two grid methods and the conjugate gradient method.

In §6.2, under some appropriate assumptions, we first generalize the two grid methods of Chapter 2 (for compact operator equations) to solve the integral equation of bounded linear operators with compact perturbations and then prove

the convergence results for these generalized two grids. The specific application of the two grid methods of §6.2 to integral equations on non-smooth boundaries is dealt with in §6.3, where a very general scheme of operator splitting is presented to gain good two grid efficiency. Some numerical experiments are carried out in §6.4, where we compare several variants of the two grid methods. The final section §6.5 is devoted to the experiments with the CG method.

6.2 General iterative schemes

Many boundary integral equations from practical applications can be characterized by a second kind integral equation of the form

$$(\mathcal{D} + \mathcal{C})u = f(s), \quad s \in [a, b], \quad (6.1)$$

where $\mathcal{D} = \mathcal{I} + \mathcal{B}$ is a bounded linear operator with bounded inverse \mathcal{D}^{-1} and \mathcal{C} is a compact operator in some Banach space X . Here we let X be the Banach space of continuous functions over $[a, b]$ with the supremum norm. For boundary integral equations on smooth boundaries (refer to Chapter 2), we may specify that $\mathcal{D} = \mathcal{I}$ and $\mathcal{C} = -\mathcal{K}$; (see (2.8)). While for equations on non-smooth boundaries (refer to Chapter 5), we consider the model equation (5.44) which is equivalent to (6.1) with $\mathcal{D} = \mathcal{I} - \mathcal{K}$ and $\mathcal{C} = -\mathcal{L}$. Here, the collocation projection method is our prime choice for solving integral equations. However, the analysis of the section will be valid for both the iterated collocation and the Nyström method.

To concentrate on the analysis only, let us adopt the notation used in §3.1 and use the setting of grids and approximate operators for simplicity of presentation. Let us denote by $\{G[l]\}_{l=1}^{\infty}$ a sequence of grids (with number of grid points $\{N_l\}_{l=1}^{\infty}$

such that $N_1 < N_2 < \dots$), on each of which the approximate solution of (6.1) is denoted by u_l and the approximate operators of \mathcal{D} and \mathcal{C} are denoted by \mathcal{D}_l and \mathcal{C}_l respectively. For the iterated collocation method (refer to §2.1), $G[l]$ represents the collection of N_l collocation points and $\mathcal{D}_l = \mathcal{D}\mathcal{P}_l$ and $\mathcal{C}_l = \mathcal{C}\mathcal{P}_l$ (for some projection operator \mathcal{P}_l); while for the Nyström method (refer to §2.2), $G[l]$ represents the union of all N_l integration nodes¹ and the operators \mathcal{D}_l and \mathcal{C}_l are defined through the composite interpolatory quadrature rule. Symbolically we write the approximate equation as

$$(\mathcal{D}_l + \mathcal{C}_l)u_l(s) = f(s), \quad s \in [a, b], \quad (6.2)$$

i.e.

$$(\mathcal{I} + \mathcal{B}_l + \mathcal{C}_l)u_l(s) = f(s), \quad s \in [a, b]. \quad (6.3)$$

where $u_l \in X$. Evaluating (6.2) at the nodes $\{s_j^l\}_1^{N_l}$ yields the linear system of size $N_l \times N_l$

$$(\mathcal{D}_l + \mathcal{C}_l)u_l(s_j^l) = f(s_j^l), \quad s_j^l \in G[l]. \quad (6.4)$$

The system (6.4) is first to be solved for the N_l unknowns $u_l(s_j^l)$ which are then used to compute $u_l(s)$ for other $s \in [a, b]$ via

$$u_l(s) = f(s) - (\mathcal{B}_l + \mathcal{C}_l)u_l(s).$$

To measure the discretization error, we may subtract (6.2) from (6.1) to obtain

$$u - u_l = (\mathcal{D}_l + \mathcal{C}_l)^{-1}(\mathcal{D}_l - \mathcal{D} + \mathcal{C}_l - \mathcal{C})u, \quad (6.5)$$

i.e.

$$\|u - u_l\| \leq \|(\mathcal{D}_l + \mathcal{C}_l)^{-1}\| \cdot \|(\mathcal{D}_l - \mathcal{D} + \mathcal{C}_l - \mathcal{C})u\|. \quad (6.6)$$

¹In general, an r point interpolatory quadrature rule is applied to each of the l subintervals in $[a, b]$ so we have $N_l = lr$.

Here in this section, we make the following assumptions (concerning (6.6)):

A1 : the first term is uniformly bounded *i.e.* $\|(\mathcal{D}_l + \mathcal{C}_l)^{-1}\| \leq c_1$;

A2 : the second term converges to zero as $l \rightarrow \infty$, $\forall u \in X$.

Following Theorem 5.7, it can be shown that the assumption **A1** is equivalent to requiring $\|\mathcal{D}_l^{-1}\| \leq c_2$ since \mathcal{C} is compact in X . We remark that of the two assumptions (i) **A1** is in general more difficult to prove; (ii) **A2** can generally be satisfied from the convergence of the interpolatory quadrature rule used. For the moment, let us assume that both **A1** and **A2** are true² and concentrate on investigating the convergence of iterative methods. For the application in the next section, we shall discuss again the two assumptions.

By varying l in (6.2), we form a sequence of approximate equations with operators $\{\mathcal{D}_l\}$ and $\{\mathcal{C}_l\}$. Suppose that we choose two integers $l = m, n$ such that $n < m$, corresponding to a fine grid $G[m]$ with N_m points and a coarse grid $G[n]$ with N_n points respectively. Then we intend to solve the equation on the operational fine grid $G[m]$

$$(\mathcal{D}_m + \mathcal{C}_m)u_m = f \tag{6.7}$$

by a two grid method *i.e.*, repeatedly using the information obtained cheaply from a solution of a residual equation on the coarse grid $G[n]$ in order to efficiently solve (6.7). Refer to [14] and Chapter 3 for related two grid ideas and implementation details. We shall now generalize the two grid ideas of Chapter 3. Here we start with the generalization of Method II.

Method II

²This implies the convergence of approximate solutions to the solution of the underlying integral equation.

To introduce the two grid method, suppose that there exists an approximation $u_m^{(\tau)}$ for the solution of (6.7), with its residual $r_m^{(\tau)} = f - (\mathcal{D}_m + C_m)u_m^{(\tau)}$. Then we propose the following smoothing step

$$\mathcal{D}_m \bar{u}_m^{(\tau)} = f - C_m u_m^{(\tau)} \quad \text{i.e.} \quad \bar{u}_m^{(\tau)} = \mathcal{D}_m^{-1}(f - C_m u_m^{(\tau)}) \quad (6.8)$$

and subsequently compute the new residual

$$\bar{r}_m^{(\tau)} = f - (\mathcal{D}_m + C_m)\bar{u}_m^{(\tau)}. \quad (6.9)$$

It can be easily shown that

$$\begin{cases} \bar{u}_m^{(\tau)} &= u_m^{(\tau)} + \mathcal{D}_m^{-1} r_m^{(\tau)}; \\ \bar{r}_m^{(\tau)} &= -C_m \mathcal{D}_m^{-1} r_m^{(\tau)}. \end{cases} \quad (6.10)$$

Now the correction equation for $\bar{r}_m^{(\tau)}$ on grid $G[n]$ is given by

$$(\mathcal{D}_n + C_n)v_n^{(\tau)} = \bar{r}_m^{(\tau)}, \quad (6.11)$$

which is solved accurately by a direct solver (Gaussian elimination with partial pivoting) for $v_n^{(\tau)}(s_j^n)$. The Nyström interpolation is then used to give the correction function $v_m^{(\tau)}(s)$ for $s = s_j^n$, $j = 1, \dots, N_m$

$$\mathcal{D}_m v_m^{(\tau)}(s) = \bar{r}_m^{(\tau)} - C_n v_n^{(\tau)} \quad \text{i.e.} \quad v_m^{(\tau)}(s) = \mathcal{D}_m^{-1}(\bar{r}_m^{(\tau)} - C_n v_n^{(\tau)}). \quad (6.12)$$

Hence our new approximation is naturally given by

$$u_m^{(\tau+1)} = \bar{u}_m^{(\tau)} + v_m^{(\tau)} = u_m^{(\tau)} + \mathcal{D}_m^{-1} r_m^{(\tau)} + v_m^{(\tau)}. \quad (6.13)$$

Expanding the right hand side of (6.13) in terms of $u_m^{(\tau)}$, $r_m^{(\tau)}$, we can obtain the iterative formula in a more standard form (refer to §3.2)

$$u_m^{(\tau+1)} = u_m^{(\tau)} + B r_m^{(\tau)} \quad (6.14)$$

where $B = \mathcal{D}_m^{-1}\{I - [I - C_n(\mathcal{D}_n + C_n)^{-1}]C_m\mathcal{D}_m^{-1}\}$. The iteration operator can be immediately given by (assume $A = \mathcal{D}_m + C_m$)

$$\begin{aligned} I - BA &= I - \mathcal{D}_m^{-1}\{I - [I - C_n(\mathcal{D}_n + C_n)^{-1}]C_m\mathcal{D}_m^{-1}\}(\mathcal{D}_m + C_m) \\ &= \mathcal{D}_m^{-1}C_m\mathcal{D}_m^{-1}C_m - \mathcal{D}_m^{-1}C_n(\mathcal{D}_n + C_n)^{-1}(\mathcal{D}_m + C_m)\mathcal{D}_m^{-1}C_m \\ &= \mathcal{D}_m^{-1}\{C_m - C_n(\mathcal{D}_n + C_n)^{-1}(\mathcal{D}_m + C_m)\}\mathcal{D}_m^{-1}C_m. \end{aligned} \quad (6.15)$$

Let us denote by $\eta_{m,n}^{\text{II}} = \|I - BA\|$ the two grid reduction factor. Then using the boundedness of \mathcal{D}_m^{-1} in (6.15), we have

$$\eta_{m,n}^{\text{II}} \leq c_3\|[C_m - C_n(\mathcal{D}_n + C_n)^{-1}(\mathcal{D}_m + C_m)]\mathcal{D}_m^{-1}C_m\|. \quad (6.16)$$

To further simplify $\eta_{m,n}^{\text{II}}$, we shall require the following lemma

LEMMA 6.1

Let $\mathcal{U}, \mathcal{V} : Y \rightarrow Y$ be linear bounded operators in some Banach space Y and $\mathcal{U}_p, \mathcal{V}_p$ two operator sequences defined on Y converging to \mathcal{U}, \mathcal{V} pointwise (i.e. satisfying $\mathcal{U}_p x \rightarrow \mathcal{U}x$ and $\mathcal{V}_p x \rightarrow \mathcal{V}x, \forall x \in Y$ as $p \rightarrow \infty$) respectively. Then the uniform boundedness of either operator sequence will guarantee the pointwise convergence $\mathcal{U}_p \mathcal{V}_p \rightarrow \mathcal{U} \mathcal{V}$ i.e. $\mathcal{U}_p \mathcal{V}_p x \rightarrow \mathcal{U} \mathcal{V}x, \forall x \in Y$ as $p \rightarrow \infty$.

Proof. Let us assume without loss of generality that $\|\mathcal{U}_p\| \leq c$. Then for each $x \in Y, y = \mathcal{V}x \in Y$ we have

$$\begin{aligned} \|\mathcal{U}_p \mathcal{V}_p x - \mathcal{U} \mathcal{V}x\| &= \|\mathcal{U}_p(\mathcal{V}_p - \mathcal{V})x + (\mathcal{U}_p - \mathcal{U})\mathcal{V}x\| \\ &\leq \|\mathcal{U}_p\| \|(\mathcal{V}_p - \mathcal{V})x\| + \|(\mathcal{U}_p - \mathcal{U})\mathcal{V}x\| \\ &\leq c\|(\mathcal{V}_p - \mathcal{V})x\| + \|(\mathcal{U}_p - \mathcal{U})y\|, \end{aligned}$$

which goes to zero as $p \rightarrow \infty$. Hence the lemma is proved. \square

Applying the lemma to terms in (6.16), we see that

$$\left. \begin{aligned} C_m \mathcal{D}_m^{-1} &\rightarrow C \mathcal{D}^{-1} \text{ pointwise as } m, n \rightarrow \infty, \\ C_n (\mathcal{D}_n + C_n)^{-1} (\mathcal{D}_m + C_m) \mathcal{D}_m^{-1} &\rightarrow C \mathcal{D}^{-1} \text{ pointwise as } m, n \rightarrow \infty. \end{aligned} \right\} (6.17)$$

Since C is compact and from the relation

$$\begin{aligned} &[C_m - C_n (\mathcal{D}_n + C_n)^{-1} (\mathcal{D}_m + C_m)] \mathcal{D}_m^{-1} \\ &= (C_m \mathcal{D}_m^{-1} - C \mathcal{D}^{-1}) + [C \mathcal{D}^{-1} - C_n (\mathcal{D}_n + C_n)^{-1} (\mathcal{D}_m + C_m) \mathcal{D}_m^{-1}], \end{aligned} \quad (6.18)$$

we therefore conclude that $\eta_{m,n}^{II} \rightarrow 0$ as $m, n \rightarrow \infty$; (refer to [11, p.8] and Theorem 1.4). Thus we have proved the following convergence result.

THEOREM 6.2

The two grid method II of (6.14) converges for sufficiently large values of m, n with $n < m$. In particular, its reduction factor satisfies

$$\lim_{m,n \rightarrow \infty} \eta_{m,n}^{II} = 0. \quad \square$$

Method I

We now generalize the Method I and then proceed to present its convergence analysis; (refer to [14, Ch.3] and Chapter 3). Method I is similar to Method II (based on (6.8)-(6.14)) except that the smoothing step (6.8) is missed out. Instead, with current approximation $u_m^{(\tau)}$, we go on to set up the correction equation for $v_m^{(\tau)}$ on $G[n]$

$$(\mathcal{D}_n + C_n) v_n^{(\tau)} = r_m^{(\tau)}, \quad (6.19)$$

in place of (6.11). Then we employ the Nyström interpolation equation to find the correction function $v_m^{(\tau)}(s)$ for $s = s_j^m, j = 1, \dots, N_m$

$$\mathcal{D}_m v_m^{(\tau)}(s) = r_m^{(\tau)} - C_n v_n^{(\tau)} \text{ i.e. } v_m^{(\tau)}(s) = \mathcal{D}_m^{-1} (r_m^{(\tau)} - C_n v_n^{(\tau)}). \quad (6.20)$$

Finally our new approximation is given by

$$u_m^{(\tau+1)} = u_m^{(\tau)} + v_m^{(\tau)}, \quad (6.21)$$

which gives rise to an iterative formula for Method I

$$u_m^{(\tau+1)} = u_m^{(\tau)} + B_1 r_m^{(\tau)}, \quad (6.22)$$

where $B_1 = \mathcal{D}_m^{-1}[\mathcal{I} - C_n(\mathcal{D}_n + C_n)^{-1}]$. The corresponding iteration operator is given by (again assume $A = \mathcal{D}_m + C_m$)

$$\begin{aligned} \mathcal{I} - B_1 A &= \mathcal{I} - \mathcal{D}_m^{-1}[\mathcal{I} - C_n(\mathcal{D}_n + C_n)^{-1}](\mathcal{D}_m + C_m) \\ &= -\mathcal{D}_m^{-1}[C_m - C_n(\mathcal{D}_n + C_n)^{-1}], \end{aligned} \quad (6.23)$$

the norm of which $\|\mathcal{I} - B_1 A\|$ cannot be shown to converge to zero as $m, n \rightarrow \infty$.

In view of the sufficient condition (3.7), let us define $\zeta_{m,n}^I = \|(\mathcal{I} - B_1 A)^2\|$. Then it is easy to verify that

$$\begin{aligned} \zeta_{m,n}^I &\leq c_4 \| [C_m - C_n(\mathcal{D}_n + C_n)^{-1}(\mathcal{D}_m + C_m)] \mathcal{D}_m^{-1} C_n \| \\ &\quad + c_5 \| [C_m - C_n(\mathcal{D}_n + C_n)^{-1}(\mathcal{D}_m + C_m)] \mathcal{D}_m^{-1} C_m \|. \end{aligned}$$

THEOREM 6.3

The two grid method I of (6.22) converges for sufficiently large values of m, n with $n < m$. In particular, its 2-step reduction factor satisfies

$$\lim_{m,n \rightarrow \infty} \zeta_{m,n}^I = 0.$$

Proof. Using Lemma 6.1 and by referring to (6.17) and (6.18), the proof immediately follows. □

For implementation of both the method I and the method II, we now present the following detailed algorithm. Here we shall require these quantities :

D_m : $N_m \times N_m$ matrix from operator \mathcal{D}_m evaluated at $G[m]$ points;

C_m : $N_m \times N_m$ matrix from operator \mathcal{C}_m evaluated at $G[m]$ points;

C_{mn} : $N_m \times N_n$ matrix from operator \mathcal{C}_n evaluated at $G[m]$ points;

A_n : $N_n \times N_n$ matrix from operator $\mathcal{A}_n = \mathcal{D}_n + \mathcal{C}_n$ evaluated at $G[n]$ points,

and vector f_m with $(f_m)_j = f(p_j)$, $p_j \in G[m]$; where D_m is usually of some sparse form depending on the boundary that defines \mathcal{D} . Then starting from an initial guess of $u_m = 0$, we can describe our general two grid algorithm GTG-1/2 as follows :

- 0) Set $r_m = f_m$, $u_m = 0$, and input TOL(tolerance) and go to step 3;
- 1) Find the residual on $G[m]$: $r_m = f_m - (D_m + C_m)u_m$;
- 2) Perform smoothing on $G[m]$: $u_m = u_m + D_m^{-1}r_m$ and $r_m = -C_m D_m^{-1}r_m$;
(This step is for Method II only)
- 3) Restrict the residual r_m to $G[n]$: $r_n = R_m^n r_m$;
- 4) Solve exactly on $G[n]$: $A_n v_n = r_n$;
- 5) Interpolate v_n to obtain v_m on $G[m]$, $v_m = D_m^{-1}(r_m - C_{mn}v_n)$;
- 6) Add on the correction v_m to u_m , $u_m = u_m + v_m$;
- 7) If $\|v_m\| \leq \text{TOL}$ exit with solution in u_m ; otherwise go to step 1.

Here the restriction operator R_m^n may be taken to be the so-called injection operator, if we choose $N_m = rN_n$ for some integer ratio r and if we are using the panel

method (piecewise constant approximations) or the Nyström method of special choices such that all $G[n]$ points form a subset of $G[m]$. But in general R_m^n represents the process of finding the residual r_n on grid $G[n]$, i.e., $r_n = f_n - A_{nm}u_m$, where A_{nm} is a $N_n \times N_m$ matrix from operator $A_m = D_m + C_m$ evaluated at $G[n]$ points. If $G[n] \not\subset G[m]$, we may also obtain the r_n values (on $G[n]$) from a simple (linear) interpolation of the r_m values.

It now remains to discuss the efficiency of both two grid methods. Inspection of the algorithms reveals that both require the solution of $D_m v = r$ for many right hand sides. As is well known, the direct inversion of D_m would require $O(N_m^3)$ operations. Therefore the generalized two grid methods do not promise to require only $O(N_m^2)$ operations, the ideal two grid efficiency (refer to [52], [58] and Chapter 3), unless the solution of the system $D_m v = r$ can be found in $O(N_m^2)$ operations. Thus the complexity of the operator \mathcal{D} is of great importance³. In the next section however, we shall see that for a particular type of problem it is possible to choose an appropriate operator \mathcal{D} in order to solve $D_m v = r$ in $O(N_m^2)$ operations, leading to practical algorithms.

6.3 Application to polygonal boundaries

Often in practice, non-compact operators in boundary integral equations may arise from either non-smooth kernels (see the N_k operator in §1.3-1.4) or non-smooth boundaries (see Chapter 5). Here we assume that the non-compactness

³We note that in [87] for a first kind integral equation, \mathcal{D} happens to be a operator of convolution kernel. Therefore, $D_m v = r$ can be solved in $O(N_m^2)$ operations when a Fast Fourier Transformation (FFT) algorithm is employed.

of the integral operator is due to the non-smoothness of the boundary. In this case, polygonal boundaries, as considered in [19], are of particular interests since integral operators on general boundaries of curved corners will have the same singular behaviour as those on polygons except for a compact perturbation; (refer to [18]).

We see from Chapter 5 that second kind integral equations on boundaries with a typical corner may be represented by (5.44) *i.e.*

$$(\mathcal{I} - \mathcal{K} - \mathcal{L})\psi(s) = V(s), \quad 0 \leq s \leq 1, \quad (6.24)$$

which characterizes the complete integral equation (5.8), where \mathcal{L} is compact in $C^0[0, 1]$. To apply the results from last section, we shall rewrite (6.24) as

$$(\mathcal{D} \div \mathcal{C})\psi(s) = V(s), \quad 0 \leq s \leq 1, \quad (6.25)$$

where $\mathcal{D} = \mathcal{I} - \mathcal{K}_\delta$, $\mathcal{C} = \mathcal{K}_\delta - \mathcal{K} - \mathcal{L}$ and $(\mathcal{K}_\delta\psi)(s) = \int_0^\delta K(\frac{s}{t})\psi(t)\frac{dt}{t}$, $0 < s \leq 1$ with $0 < \delta \leq 1$ fixed, where \mathcal{D}^{-1} exists since $\|\mathcal{K}_\delta\| \leq \|\mathcal{K}\| < 1$. This operator \mathcal{K}_δ is somewhat similar to that defined in [57] and [88]. For $\delta > 0$, $\mathcal{K}_\delta - \mathcal{K}$ will be compact because of the continuity of its kernel, implying that \mathcal{C} is compact. Therefore (6.25) falls into the class represented by (6.1).

For the numerical solution of (6.25), we shall use the collocation methods as introduced in §5.2. In order to set up a projection operator on $G[l]$, we can follow (5.32) of §5.2.2 to obtain $\mathcal{P}_l : C^0[0, 1] \div S^{l,r} \rightarrow S^{l,r}$. Using \mathcal{P}_l , we may define our product integration approximation to ψ in (6.25) as follows

$$(\mathcal{D}_l \div \mathcal{C}_l)\psi_l = V, \quad (6.26)$$

where $\mathcal{D}_l = \mathcal{I} - \mathcal{K}_\delta\mathcal{P}_l$ and $\mathcal{C}_l = \mathcal{C}\mathcal{P}_l$; (refer to (5.34)). To give an error analysis for (6.26), we can refer back to (6.6), which requires both the stability (A1) and

The two assumptions A1 and A2 are both satisfied.

We are now in a position to apply the two-grid methods of the results of the last section. The convergence of both variants can be ensured in this setting, following the last section. However, our main concern here is to investigate the overall efficiency of these methods. Let us first look at the problem of choosing a suitable parameter δ . Obviously, for any fixed $\delta > 0$, the cost of inverting \mathcal{D}_m will be asymptotically of order $cN_m^3 = O(N_m^3)$ operations, though constant c may be quite small (proportional to $\delta^{3/q}$ as $\delta^{1/q}$ approximates the number of terms in \mathcal{D}_m). For example if $\delta = 0.05$, $c \approx 1.25 \times 10^{-4}$ for $q = 1$ (uniform mesh) and $c \approx 0.106$ for $q = 4$ (non-uniform mesh). Also the size of the linear

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$$\mathcal{D}_l^{-1} = (\mathcal{I} - \mathcal{K}_\delta \mathcal{P}_l)^{-1} = \mathcal{I} + \mathcal{K}_\delta (\mathcal{I} - \mathcal{P}_l \mathcal{K}_\delta)^{-1} \mathcal{P}_l$$

the operator identity (5.40)

to show $\|(\mathcal{D}_l + \mathcal{C}_l)^{-1}\| \leq c$, we only need to consider the quantity $\|\mathcal{D}_l^{-1}\|$. From the consistency (A2) results. In view of Theorem 5.7, for the stability result (i.e.

system associated with \mathcal{D}_m increases as the mesh grading exponent q increases for the same δ . Therefore, the theoretical complexity of our two grid methods is $O(N_m^3)$, rather than $O(N_m^2)$ which was the case with smooth operator equations of Chapter 3. Nevertheless, efficiency of order $O(N_m^2)$ may be practically restored and observed because of the following two observations : (i) system $\mathcal{D}_m v = r$ may be solved efficiently by a secondary iterative process; see [86] and [87]; (ii) although theories predict that the convergence rate of two grid methods goes to zero as $m, n \rightarrow \infty$, in practice, we only require it to be less than 1 for convergence and often very reasonable convergence can be observed once $m, n > n_0$ (typically $n_0 \approx 40$). The effect of (ii) is now expanded in more details. Essentially we shall make special choices of \mathcal{D} in order to solve $\mathcal{D}_m v = r$ more efficiently.

Minimum δ -Algorithm (M δ)

Suppose that N^* is the largest order of linear system one particular computer can handle. Then using r th order piecewise polynomials on a graded mesh (with grading exponent q), we define

$$\delta^* = \left(\frac{1}{n^*}\right)^q, \quad n^* = \text{INT} \left[\frac{N^*}{r} \right] \quad (6.27)$$

and choose $\delta = \delta^*$, where $\text{INT}[\cdot]$ denotes the integer part of a number. With such a choice of δ for setting up (6.25), we then adopt the first modified collocation method (§5.2.3) with $i = i^* = 1$. For any $m \leq n^*$, the projection operator $\bar{\mathcal{P}}_m$ on $[0, \eta_1^m]$ is based on piecewise constant approximations. Therefore the matrix D_m associated with operator \mathcal{D}_m will be of the form

$$D_m = \begin{bmatrix} \times & & & & \\ & \times & & & \\ & & \times & & \\ & & & \ddots & \\ \times & & & & \times \end{bmatrix} \quad (6.28)$$

the inverse of which is found in $O(N_m)$ operations and has the same sparse structure, given by

$$(D_m^{-1})_{ij} = \begin{cases} \frac{1}{(D_m)_{ij}}, & i = j, \\ 0, & i \neq j, \quad j \neq 1, \\ -\frac{(D_m)_{ij}}{(D_m)_{ii}(D_m)_{11}}, & i > 1, \quad j = 1. \end{cases} \quad (6.29)$$

Thus the complexity of two grid methods is restored to $O(N_m^2)$ operations. Actually, the idea may also be specialized. For given sufficiently large $m, n : n_0 \leq m, n \leq n^*$, we may make this choice for δ

$$\delta = \bar{\delta} = \left(\frac{1}{m}\right)^q, \quad (6.30)$$

maintaining the complexity of two grid methods at $O(N_m^2)$ operations.

We note that the choice for δ^* in (6.27) may be generalized to

$$\delta^* = \left(\frac{\tau}{n^*}\right)^q$$

where $\tau \geq 1$. Further we may use the piecewise polynomial $S_{\tau}^{m,\tau}$ to define our collocation projection approximations; (refer to §5.2.3). The matrix D_m associated with operator \mathcal{D}_m is now of the form

$$D_m = \begin{bmatrix} A_1 & 0 \\ A_2 & I \end{bmatrix}$$

where A_1 is a $\tau \times \tau$ full matrix, A_2 is a $(N_m - \tau) \times \tau$ matrix and I is the $(N_m - \tau) \times (N_m - \tau)$ unit matrix. The inverse of D_m can be shown to be given by

$$D_m^{-1} = \begin{bmatrix} A_1^{-1} & 0 \\ -A_2 A_1^{-1} & I \end{bmatrix}.$$

The work for computing A_1^{-1} is $O(\tau^3)$ and the work for the multiplication $A_2 A_1^{-1}$ is $O(N_m \tau^2)$. Therefore we only require $O(N_m)$ operations to calculate D_m^{-1} if we fix τ . The case for the extreme choice $\tau = 1$ is discussed in (6.27)-(6.30).

Intermediate Operator Algorithm (IO)

Let us now adopt the second modified collocation method of §5.2.3 with $\ell = 0$. To this end, we rewrite (6.25) as

$$(\mathcal{I} - \mathcal{J})\psi(s) = V(s), \quad 0 \leq s \leq 1, \quad (6.31)$$

where $\mathcal{J} = \mathcal{K} + \mathcal{L}$. Following (5.50), we first approximate (6.31) by an intermediate operator equation

$$(\mathcal{I} - \mathcal{J}_\varepsilon)\psi_\varepsilon = V, \quad (6.32)$$

with $(\mathcal{J}_\varepsilon \psi)(s) = \int_\varepsilon^1 K(\frac{s}{t})\psi(t)\frac{dt}{t} + (\mathcal{L}\psi)(s)$, $\varepsilon(m) = (\frac{1}{m})^q$ and $m \geq n_0$. Since \mathcal{J}_ε is now a compact operator, we may solve (6.32) by unmodified two grid methods of Chapter 3. That is, we employ the two grid methods of last section with the choice of $\mathcal{D} = \mathcal{I}$ and $\mathcal{C} = -\mathcal{J}_\varepsilon$. A complexity of $O(N_m^2)$ operations may be expected. Refer to [14] and §3.3 for algorithmic details.

6.4 Numerical experiments

Here we solve the example given in §5.3 by various two grid methods discussed in the previous section. We demonstrate and compare their convergence and effi-

ciency. In all the following experiments, iterative solutions are terminated when a residual in root mean square norm (RMS) less than TOL is obtained. The choice for TOL should be based on expected level of discretization error and will be discussed in more details. The number of iterations required to achieve the desired accuracy is denoted by "STEPS" and the corresponding cpu seconds used by Prime-750 by "CPU". A direct solver requires CPU =0.2, 5.0 and 130.0 respectively for solving a linear system of order 36×36 , 108×108 and 324×324 . We shall adopt the consistent notation among all tables such that "q" denotes the mesh grading exponent, "METHOD" distinguishes "V.I" for variant I and "V.II" for variant II of two grid methods and "*" means no convergence. Throughout the section, we shall use for numerical solutions the iterated collocation approximations based on both piecewise constant and piecewise linear approximations (§6.3). Therefore, orders of convergence of both approximations are $O(h_m^{1/2})$ with uniform meshes ($q = 1$); while the graded meshes with $q \geq 4$ and $q \geq 8$ respectively should restore convergence orders to $O(h_m^2)$ for piecewise constant and $O(h_m^4)$ for piecewise linear approximations.

As with all iterative methods, the stopping criterion has a great effect on the actual efficiency of the methods. Ideally we would like to stop our iterations whenever the errors are below the level of the discretization error as in general there is little to be gained by solving the discrete boundary element equations to levels of accuracy far smaller than the underlying discretization error $\|u - u_n\|$. The precise knowledge of the discretization error is in general not available, except that in our case the error is of the form $O(n^{-\alpha})$ where $\alpha = 1/2, 2, 4$ for example depending on the discretization method and the smoothness of the solution (or

the choice of the grading exponent q). For our test problem, we can obtain some knowledge of the exact discretization error by solving the system directly. We find that the following choice for the tolerance TOL is appropriate so that it is below our observed level of the discretization error : (i) with $q = 1$, choose $\text{TOL}=10^{-2}$ for any $N_n \leq 324$; (ii) with $q = 4$, choose $\text{TOL}=10^{-3}$ for $N_n = 36$, $\text{TOL}=10^{-4}$ for $N_n = 108$ and $\text{TOL}=10^{-5}$ for $N_n = 324$; (iii) with $q = 8$, choose $\text{TOL}=10^{-4}$ for $N_n = 36$, $\text{TOL}=10^{-5}$ for $N_n = 108$ and $\text{TOL}=10^{-6}$ for $N_n = 324$.

In Tables 6.1-6.2, we solve the integral equation by the so-called direct two grid methods. By 'direct' we mean the 'unmodified' variants *i.e.* two grid methods applied to equation (6.31). We observe that two grid methods converge in all cases and in particular convergence is faster as N_m, N_n increase. Since the integral operator $\mathcal{J} = \mathcal{K} + \mathcal{L}$ involved here is known to be non-compact, we are unable to justify theoretically the convergence of direct two grid methods. Results from Tables 6.1-6.2 show that the direct two grid methods converge at reasonably fast rates. However in the 3D case, the slowing down in convergence due to the presence of non-compact operators has been observed in [15] and [17].

In Tables 6.3-6.4, we experiment with the general iterative schemes for two grid methods (§6.2-6.3) with a fixed cut δ around the corner ($s = 0$). To compare, we choose two different cuts $\delta_1 = (\frac{1}{6})^q$ and $\delta_2 = (\frac{1}{12})^q$ (notice the dependence upon the mesh grading exponent q). As expected, convergence of two grid methods with the larger cut δ_1 is faster than that of the smaller cut δ_2 but at the same time the computational cost (*e.g.* in computing D_m^{-1}) associated with δ_1 is greater than that with δ_2 . Comparing Tables 6.3-6.4 with Tables 6.1-6.2 respectively, we see that the convergence in the former two is overall much faster than that in

the latter two but CPU times are also greater in the former. Similar tests with two grid methods using the general iterative scheme (*i.e.* using a general δ) for potential flow problems on non-smooth boundary can be found in [86] and [88], where $\delta = \frac{1}{10}$ is chosen. See also [57].

In Tables 6.5-6.6, we present the results of solving the same integral equation by the Minimum δ -algorithm (§6.3). Here on the PRIME-750, the minimum δ is chosen to be $\delta^* = (\frac{1}{100})^q$ depending on the exponent q . We also present the results from the comparable choice $\bar{\delta} = (\frac{1}{N_m})^q$. Finally in Tables 6.7-6.8, results are obtained from applying the IO algorithm (§6.3). The intermediate corner cut is indicated by $\varepsilon(N_m) = (\frac{1}{N_m})^q$. Numbers in Tables 6.5-6.8 compare favorably with those of previous tables.

In conclusion, we favour the use of algorithms $M\delta$ and IO from both the theoretical and the practical points of view.

6.5 Application of the conjugate gradient method

Having looked into two grid methods for solving non-smooth integral equations, we now consider the application of the conjugate gradient (CG) method, as introduced in Chapter 4. Thus the study of iterative methods would be more complete.

As is well known, the eigenvalues of a compact operator may cluster at one point (zero); (refer to Theorem 4.3). But for eigenvalues of a non-compact operator, such a simple clustering pattern may not be present. It might be true that eigenvalues of a non-compact operator (only due to non-smooth boundaries) do not accumulate at any point of an interval; (refer to Lemma 5.5). This may

suggest that the use of the CG method for the solution of the linear systems resulting from discretization of such non-smooth operator equations is not appropriate although the method converges for any linear system asymptotically (provided that the round off error is sufficiently small).

However it is usually true that a non-compact operator is approximated by a sequence of discrete compact operators and the approximate eigenvalue spectra of these discrete compact operators often do possess a simple clustering pattern. Therefore the CG method should not entirely be ruled out as an efficient iterative method for solving non-compact integral operator equations.

We have observed, for our particular problem, that unlike the case of compact operators the number O_N of eigenvalues outside the clustering region increases as N increases. The difference in clustering behaviour would indicate that the conjugate gradient method may lose its fixed step convergence property. However for a given value of N the number O_N of eigenvalues outside a given region is relatively small. Hence the present conjugate gradient method may still prove to be efficient as a practical fast solver. Below we solve the same model problem as in §6.4 using the CG method (Chapter 4) and present the related details.

In Figs.6.1-6.2, we plot the approximate eigenvalue spectra of the non-compact operator κ plus an identity operator \mathcal{I} , *i.e.* $\mathcal{A} = \mathcal{I} - \kappa$ and its normal operator $\mathcal{B} = \mathcal{A}\mathcal{A}^*$, using the piecewise constant approximations. While in Figs.6.3-6.4, we plot the corresponding approximate spectra from using piecewise linears. For each figure, we have computed the eigenvalues of three discrete cases with $N = 50, 150$ and 300 collocation points respectively. From these figures (6.1-6.4), we can observe the clear clustering patterns of eigenvalue distribution around the point

$\lambda = 1$. Recall the convergence analysis of the CG method discussed in Chapter 4. There we claim that convergence of the CG method is very fast whenever eigenvalues cluster. This certainly predicts a good efficiency of the CG method when applied to our model problem. Hence we adopt the **ALGORITHM – conjugate gradients** of §4.2 for numerical solutions.

In Tables 6.9-6.10, we list the results obtained from using the CG method for both the piecewise constant and the piecewise linear approximations. The tests are again carried out on PRIME 750 with the usual double precision arithmetic (with around 14 significant figures). The stopping criterion is as chosen in §6.4. We note that the CG method is quite fast for the case of uniform meshes ($q = 1$) and generally slow for the case of non-uniform meshes ($q > 1$ i.e. when close to the non-compact operator). Viewing the performances of the CG method (Tables 6.9-6.10) as well as two grid methods (Tables 6.1-6.8), we may conclude that all iterative methods⁵ are quite efficient in terms of number of steps to achieve the required accuracy and effective in reducing the solution time for linear systems involved. In summary, two grid methods are more efficient than the CG method as is the case with solving smooth integral equations (Chapters 3-4). To further improve the CG method, preconditioning techniques may be potentially important. However much theoretical study is needed towards the development of such preconditioners.

⁵provided that the discretization method is of low order for the present CG method.

Table 6.1: Direct two grid methods for the piecewise constant case.

| q | METHOD | Fine[m] | Coarse[n] | STEPS | CPU |
|-----|--------|---------|-----------|-------|------|
| 1 | V.I | 324 | 12 | 1 | 1.5 |
| | | | 36 | 1 | 1.9 |
| | | | 108 | 1 | 7.5 |
| | | 108 | 12 | 1 | 0.2 |
| | | | 36 | 1 | 0.5 |
| | | | 108 | 1 | 0.2 |
| | V.II | 324 | 12 | 1 | 2.9 |
| | | | 36 | 1 | 3.3 |
| | | | 108 | 1 | 8.9 |
| | | 108 | 12 | 1 | 0.4 |
| 36 | | | 1 | 0.6 | |
| 108 | | | 1 | 0.6 | |
| 4 | V.I | 324 | 12 | 12 | 17.6 |
| | | | 36 | 4 | 6.7 |
| | | | 108 | 2 | 9.4 |
| | | 108 | 12 | 4 | 0.8 |
| | | | 36 | 2 | 0.7 |
| | | | 108 | 2 | 0.7 |
| | V.II | 324 | 12 | 8 | 22.4 |
| | | | 36 | 3 | 9.1 |
| | | | 108 | 2 | 12.1 |
| | | 108 | 12 | 3 | 1.0 |
| 36 | | | 2 | 1.0 | |
| 108 | | | 2 | 1.0 | |

Table 6.2: Direct two grid methods for the piecewise linear case.

| q | METHOD | Fine[m] | Coarse[n] | STEPS | CPU |
|-----|--------|---------|-----------|-------|------|
| 1 | V.I | 324 | 12 | 1 | 1.5 |
| | | | 36 | 1 | 2.0 |
| | | | 108 | 1 | 7.8 |
| | | 108 | 12 | 1 | 0.2 |
| | | | 36 | 1 | 0.5 |
| | | | 108 | 1 | 0.2 |
| | V.II | 324 | 12 | 1 | 2.9 |
| | | | 36 | 1 | 3.4 |
| | | | 108 | 1 | 9.2 |
| | | 108 | 12 | 1 | 0.4 |
| 36 | | | 1 | 0.7 | |
| 108 | | | 1 | 0.7 | |
| 8 | V.I | 324 | 12 | 18 | 32.9 |
| | | | 36 | 6 | 13.3 |
| | | | 108 | 2 | 12.1 |
| | | 108 | 12 | 11 | 3.9 |
| | | | 36 | 3 | 1.9 |
| | | | 108 | 3 | 1.9 |
| | V.II | 324 | 12 | 13 | 37.0 |
| | | | 36 | 4 | 12.5 |
| | | | 108 | 2 | 13.0 |
| | | 108 | 12 | 6 | 2.1 |
| 36 | | | 3 | 1.5 | |
| 108 | | | 3 | 1.5 | |

Table 6.3: General iterative schemes for the piecewise constant case (fixed δ).

| q | δ | METHOD | Fine[m] | Coarse[n] | STEPS | CPU | |
|------|-------------------------------|--------|---------|-----------|-------|------|-----|
| 1 | $\frac{1}{6}$ | V.I | 324 | 12 | 4 | 7.5 | |
| | | | | 36 | 4 | 8.2 | |
| | | | | 108 | 4 | 15.0 | |
| | | V.II | 324 | 12 | 3 | 11.8 | |
| | | | | 36 | 3 | 12.4 | |
| | | | | 108 | 3 | 18.8 | |
| | V.II | 108 | 12 | 3 | 1.4 | | |
| | | | 36 | 3 | 1.7 | | |
| | | | | | | | |
| | $\frac{1}{12}$ | V.I | 324 | 12 | 4 | 6.5 | |
| | | | | 36 | 4 | 7.2 | |
| | | | | 108 | 4 | 14.0 | |
| | | | V.I | 108 | 12 | 4 | 0.8 |
| | | | | | 36 | 4 | 1.2 |
| | | | | | | | |
| V.II | | 324 | 12 | 3 | 10.0 | | |
| | | | 36 | 3 | 10.6 | | |
| | | | 108 | 3 | 17.0 | | |
| V.II | | 108 | 12 | 3 | 1.2 | | |
| | | | 36 | 3 | 1.5 | | |
| | | | | | | | |
| 4 | $\left(\frac{1}{6}\right)^4$ | V.I | 324 | 12 | 10 | 17.4 | |
| | | | | 36 | 10 | 18.9 | |
| | | | | 108 | 10 | 28.4 | |
| | | V.I | 108 | 12 | 8 | 1.7 | |
| | | | | 36 | 8 | 2.3 | |
| | | | | | | | |
| | | V.II | 324 | 12 | 10 | 37.8 | |
| | | | | 36 | 10 | 39.2 | |
| | | | | 108 | 10 | 48.5 | |
| | V.II | 108 | 12 | 7 | 3.1 | | |
| | | | 36 | 7 | 3.6 | | |
| | | | | | | | |
| | $\left(\frac{1}{12}\right)^4$ | V.I | 324 | 12 | 10 | 15.9 | |
| | | | | 36 | 10 | 17.4 | |
| | | | | 108 | 10 | 27.1 | |
| | | V.I | 108 | 12 | 8 | 1.6 | |
| | | | | 36 | 8 | 2.2 | |
| | | | | | | | |
| V.II | | 324 | 12 | 10 | 33.1 | | |
| | | | 36 | 10 | 34.2 | | |
| | | | 108 | 10 | 43.7 | | |
| V.II | 108 | 12 | 7 | 2.7 | | | |
| | | 36 | 7 | 3.2 | | | |
| | | | | | | | |

Table 6.4: General iterative schemes for the piecewise linear case (fixed δ).

| q | δ | METHOD | Fine[m] | Coarse[n] | STEPS | CPU | |
|------|-------------------------------|--------|---------|-----------|-------|------|-----|
| 1 | $\frac{1}{6}$ | V.I | 324 | 12 | 1 | 2.4 | |
| | | | | 36 | 1 | 2.8 | |
| | | | | 108 | 1 | 8.3 | |
| | | V.II | 324 | 12 | 1 | 4.5 | |
| | | | | 36 | 1 | 5.0 | |
| | | | | 108 | 1 | 10.4 | |
| | V.II | 108 | 12 | 1 | 0.5 | | |
| | | | 36 | 1 | 0.8 | | |
| | | | | | | | |
| | $\frac{1}{12}$ | V.I | 324 | 12 | 4 | 6.3 | |
| | | | | 36 | 1 | 2.1 | |
| | | | | 108 | 1 | 2.0 | |
| | | | V.I | 108 | 12 | 4 | 0.8 |
| | | | | | 36 | 1 | 0.5 |
| | | | | | | | |
| V.II | | 324 | 12 | 3 | 10.0 | | |
| | | | 36 | 1 | 3.9 | | |
| | | | 108 | 1 | 9.3 | | |
| | | V.II | 108 | 12 | 3 | 1.2 | |
| | | | | 36 | 1 | 0.7 | |
| | | | | | | | |
| S | $\left(\frac{1}{6}\right)^S$ | V.I | 324 | 12 | * | * | |
| | | | | 36 | 5 | 9.6 | |
| | | | | 108 | 2 | 10.4 | |
| | | V.I | 108 | 12 | * | * | |
| | | | | 36 | 3 | 1.0 | |
| | | | | | | | |
| | | V.II | 324 | 12 | * | * | |
| | | | | 36 | 4 | 16.2 | |
| | | | | 108 | 2 | 14.5 | |
| | V.II | | 108 | 12 | * | * | |
| | | | | 36 | 3 | 1.7 | |
| | | | | | | | |
| | $\left(\frac{1}{12}\right)^S$ | V.I | 324 | 12 | * | * | |
| | | | | 36 | * | * | |
| | | | | 108 | 2 | 9.6 | |
| | | V.I | 108 | 12 | * | * | |
| | | | | 36 | * | * | |
| | | | | | | | |
| V.II | | 324 | 12 | * | * | | |
| | | | 36 | 6 | 20.6 | | |
| | | | 108 | 2 | 13.1 | | |
| | V.II | 108 | 12 | * | * | | |
| | | | 36 | * | * | | |
| | | | | | | | |

Table 6.5: Minimum δ -algorithm (M δ) for the piecewise constant case.

| q | δ | METHOD | Fine[m] | Coarse[n] | STEPS | CPU |
|------|----------|---------------------|---------------------|-----------|-------|------|
| 1 | 1/400 | V.I | 324 | 12 | 1 | 1.5 |
| | | | | 36 | 1 | 1.9 |
| | | | | 108 | 1 | 7.5 |
| | | V.II | 108 | 12 | 1 | 0.2 |
| | | | | 36 | 1 | 0.5 |
| | | | | 324 | 12 | 1 |
| | V.II | 324 | 12 | 1 | 2.3 | |
| | | | 36 | 1 | 3.3 | |
| | | | 108 | 1 | 8.9 | |
| | V.II | 108 | 12 | 1 | 0.4 | |
| | | | 36 | 1 | 0.6 | |
| | | | 1/324 | V.I | 324 | 12 |
| 36 | 1 | 1.9 | | | | |
| 108 | 1 | 7.5 | | | | |
| V.II | 108 | 12 | | 1 | 0.2 | |
| | | 36 | | 1 | 0.5 | |
| | | 324 | | 12 | 1 | 2.9 |
| V.II | 324 | 12 | 1 | 2.9 | | |
| | | 36 | 1 | 3.3 | | |
| | | 108 | 1 | 8.9 | | |
| V.II | 108 | 12 | 1 | 0.4 | | |
| | | 36 | 1 | 0.6 | | |
| | | 4 | $(\frac{1}{400})^4$ | V.I | 324 | 12 |
| 36 | 4 | | | | | 6.7 |
| 108 | 2 | | | | | 9.5 |
| V.II | 108 | | | 12 | 4 | 0.8 |
| | | | | 36 | 2 | 0.7 |
| | | | | 324 | 12 | 8 |
| V.II | 324 | | 12 | 8 | 22.5 | |
| | | | 36 | 3 | 9.1 | |
| | | | 108 | 2 | 12.2 | |
| V.II | 108 | | 12 | 3 | 1.0 | |
| | | | 36 | 2 | 1.0 | |
| | | | $(\frac{1}{324})^4$ | V.I | 324 | 12 |
| 36 | 4 | 6.7 | | | | |
| 108 | 2 | 9.5 | | | | |
| V.II | 108 | 12 | | 4 | 0.8 | |
| | | 36 | | 2 | 0.7 | |
| | | 324 | | 12 | 8 | 22.5 |
| V.II | 324 | 12 | 8 | 22.5 | | |
| | | 36 | 3 | 9.1 | | |
| | | 108 | 2 | 12.2 | | |
| V.II | 108 | 12 | 8 | 2.7 | | |
| | | 36 | 3 | 1.4 | | |
| | | $(\frac{1}{108})^4$ | V.I | 324 | 12 | 12 |
| 36 | 4 | | | | 6.7 | |
| 108 | 2 | | | | 9.5 | |
| V.II | 108 | | 12 | 4 | 0.8 | |
| | | | 36 | 2 | 0.7 | |
| | | | 324 | 12 | 8 | 22.5 |
| V.II | 324 | 12 | 8 | 22.5 | | |
| | | 36 | 3 | 9.1 | | |
| | | 108 | 2 | 12.2 | | |
| V.II | 108 | 12 | 8 | 2.7 | | |
| | | 36 | 3 | 1.4 | | |

Table 6.6: Minimum δ -algorithm ($M\delta$) for the piecewise linear case.

| q | δ | METHOD | Fine[m] | Coarse[n] | STEPS | CPU |
|---------------------|---------------------|--------|---------|-----------|-------|------|
| 1 | 1/400 | V.I | 324 | 12 | 2 | 3.0 |
| | | | | 36 | 1 | 1.9 |
| | | | | 108 | 1 | 7.4 |
| | | V.II | 324 | 12 | 2 | 5.7 |
| | | | | 36 | 1 | 3.3 |
| | | | | 108 | 1 | 8.7 |
| | 1/324 | V.I | 324 | 12 | 2 | 3.0 |
| | | | | 36 | 1 | 1.9 |
| | | | | 108 | 1 | 7.4 |
| | | V.II | 324 | 12 | 2 | 5.7 |
| | | | | 36 | 1 | 3.3 |
| | | | | 108 | 1 | 8.6 |
| 1/108 | V.I | 108 | 12 | 2 | 0.4 | |
| | | | 36 | 1 | 0.5 | |
| | | | 108 | 2 | 0.7 | |
| | V.II | 108 | 12 | 2 | 0.7 | |
| | | | 36 | 1 | 0.6 | |
| | | | 108 | 2 | 0.7 | |
| 8 | $(\frac{1}{400})^8$ | V.I | 324 | 12 | † | † |
| | | | | 36 | † | † |
| | | | | 108 | 2 | 9.4 |
| | | V.II | 324 | 12 | † | † |
| | | | | 36 | 4 | 1.2 |
| | | | | 108 | 2 | 12.1 |
| | $(\frac{1}{324})^8$ | V.I | 324 | 12 | † | † |
| | | | | 36 | † | † |
| | | | | 108 | 2 | 9.4 |
| | | V.II | 324 | 12 | † | † |
| | | | | 36 | 4 | 1.2 |
| | | | | 108 | 2 | 12.1 |
| $(\frac{1}{108})^8$ | V.I | 108 | 12 | † | † | |
| | | | 36 | 4 | 1.2 | |
| | | | 108 | 2 | 12.1 | |
| | V.II | 108 | 12 | † | † | |
| | | | 36 | 2 | 1.0 | |
| | | | 108 | 2 | 1.0 | |

Table 6.7: Intermediate operator algorithm (IO) for the piecewise constant case.

| q | METHOD | Fine[m] | Coarse[n] | STEPS | CPU |
|----|--------|---------|-----------|-------|------|
| 1 | V.I | 324 | 12 | 1 | 1.5 |
| | | | 36 | 1 | 1.9 |
| | | | 108 | 1 | 7.3 |
| | | 108 | 12 | 1 | 0.2 |
| | | | 36 | 1 | 0.5 |
| | | | 108 | 1 | 0.2 |
| | V.II | 324 | 12 | 1 | 2.8 |
| | | | 36 | 1 | 3.2 |
| | | | 108 | 1 | 8.6 |
| | | 108 | 12 | 1 | 0.4 |
| 4 | V.I | 324 | 12 | 12 | 16.9 |
| | | | 36 | 4 | 6.4 |
| | | | 108 | 2 | 9.2 |
| | | 108 | 12 | 4 | 0.7 |
| | | | 36 | 2 | 0.7 |
| | | | 108 | 2 | 0.7 |
| | V.II | 324 | 12 | 8 | 21.9 |
| | | | 36 | 3 | 8.9 |
| | | | 108 | 2 | 11.9 |
| | | 108 | 12 | 3 | 1.0 |
| 36 | 12 | 2 | 1.0 | | |

Table 6.8: Intermediate operator algorithm (IO) for the piecewise linear case.

| q | METHOD | Fine[m] | Coarse[n] | STEPS | CPU |
|---|--------|---------|-----------|-------|------|
| 1 | V.I | 324 | 12 | 1 | 1.6 |
| | | | 36 | 1 | 2.1 |
| | | | 108 | 1 | 7.8 |
| | | 108 | 12 | 1 | 0.2 |
| | | | 36 | 1 | 0.5 |
| | | | 108 | 1 | 9.2 |
| | V.II | 324 | 12 | 1 | 2.9 |
| | | | 36 | 1 | 3.4 |
| | | 108 | 12 | 1 | 0.4 |
| | | | 36 | 1 | 0.7 |
| 8 | V.I | 324 | 12 | 18 | 27.0 |
| | | | 36 | 6 | 10.6 |
| | | | 108 | 2 | 10.2 |
| | | 108 | 12 | 11 | 2.2 |
| | | | 36 | 3 | 1.1 |
| | | | 108 | 2 | 12.8 |
| | V.II | 324 | 12 | 13 | 36.8 |
| | | | 36 | 4 | 12.5 |
| | | 108 | 12 | 6 | 2.1 |
| | | | 36 | 3 | 1.5 |

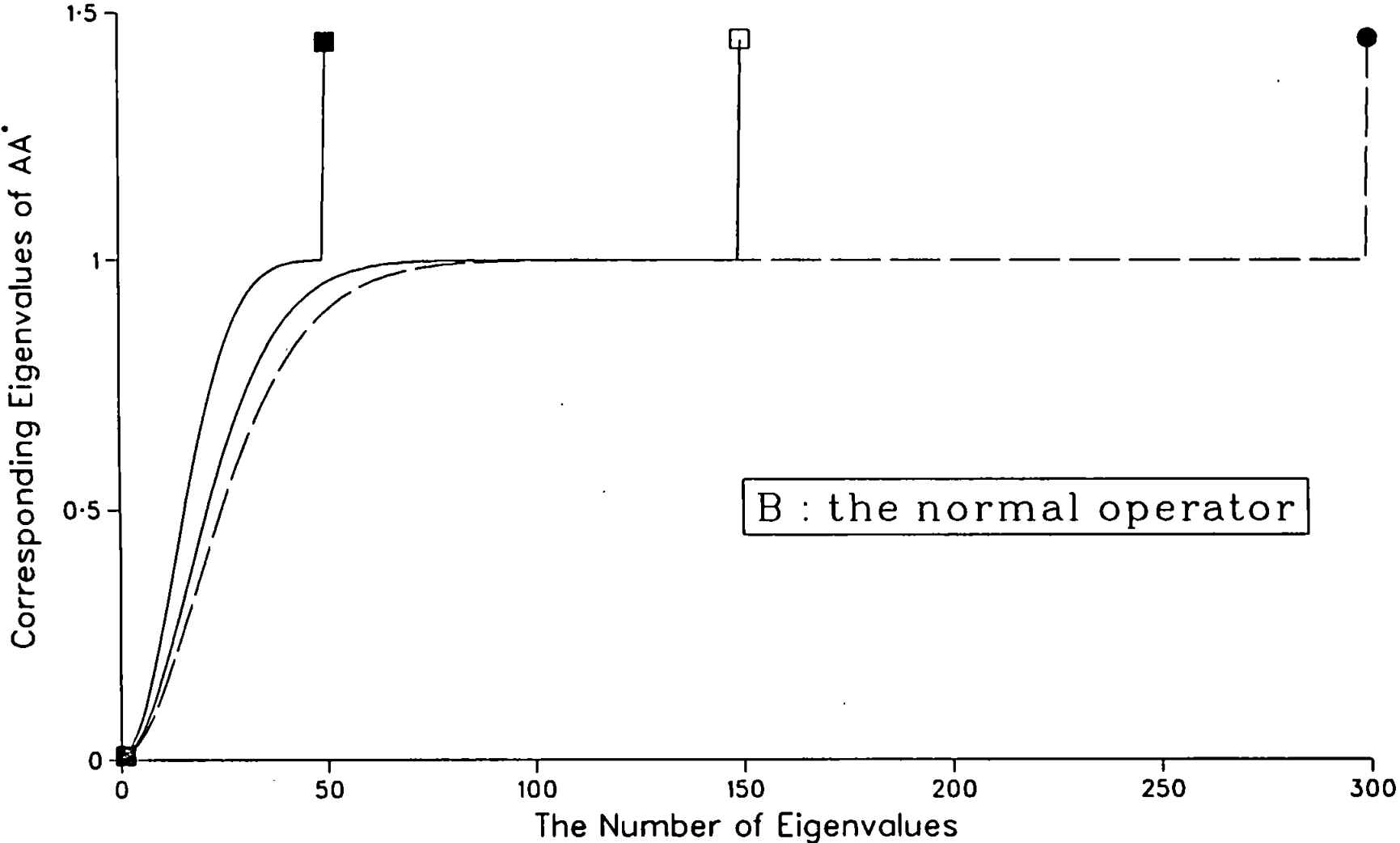
Table 6.9: The CG method with piecewise constant approximations (CPU times).

| q | Size N | Number of CG Steps | CPU Seconds |
|---|--------|--------------------|-------------|
| 1 | 36 | 5 | 0.2 |
| | 108 | 5 | 1.8 |
| | 324 | 5 | 15.6 |
| 4 | 36 | 15 | 0.6 |
| | 108 | 29 | 5.2 |
| | 324 | 42 | 131.3 |

Table 6.10: The CG method with piecewise linear approximations (CPU times).

| q | Size N | Number of CG Steps | CPU Seconds |
|---|--------|--------------------|-------------|
| 1 | 36 | 5 | 0.2 |
| | 108 | 5 | 1.8 |
| | 324 | 5 | 16.2 |
| 8 | 36 | 31 | 1.4 |
| | 108 | 57 | 20.1 |
| | 324 | 89 | 291.0 |

Fig.6.4 Approximate Eigenvalue Spectrum of $B = AA^*$ [constants, $q=4$]



With Π_n so chosen, the global convergence of the collocation solution may be given below.

THEOREM 2.1

Let r be a non-negative integer. Suppose $\phi \in C^r$. Then we have

$$\|\phi - \phi_n\| = O(h_n^r).$$

Proof. Following (2.5), we only need to show that

$$\|\phi - \mathcal{P}_n\phi\| = O(h_n^r).$$

This however follows from the interpolation theory for $\phi \in C^r$; refer to [16, Ch.3].

Thus the proof is complete. □

However the solution ϕ is generally non-smooth whenever kernel $K(s, t)$ is weakly singular; (refer to (2.8) and see [48]). Suppose that ϕ has a singularity at point $s = a$. Then we may have to employ suitable non-uniform meshes Π_n (often referred to as the *graded meshes*) i.e.

$$\eta_i = a + \left(\frac{i}{n}\right)^q \cdot (b - a), \quad i = 0, \dots, n, \quad (2.16)$$

with $q \geq 1$ in order to maintain the convergence order of $O(h_n^r)$. To give some basic idea of the approach, we now give the following result.

THEOREM 2.2

Suppose $\phi = A(s - a)^\beta \in C$ where $0 < \beta < 1$ and A is some constant. Then using the graded mesh Π_n as defined by (2.16) with $q \geq r/\beta$, we have

$$\|\phi - \phi_n\| = O(h_n^r). \quad (2.17)$$

Fig.6.1 Approximate Eigenvalue Spectrum of $A = (I - K)$ [constants, $q=1$]

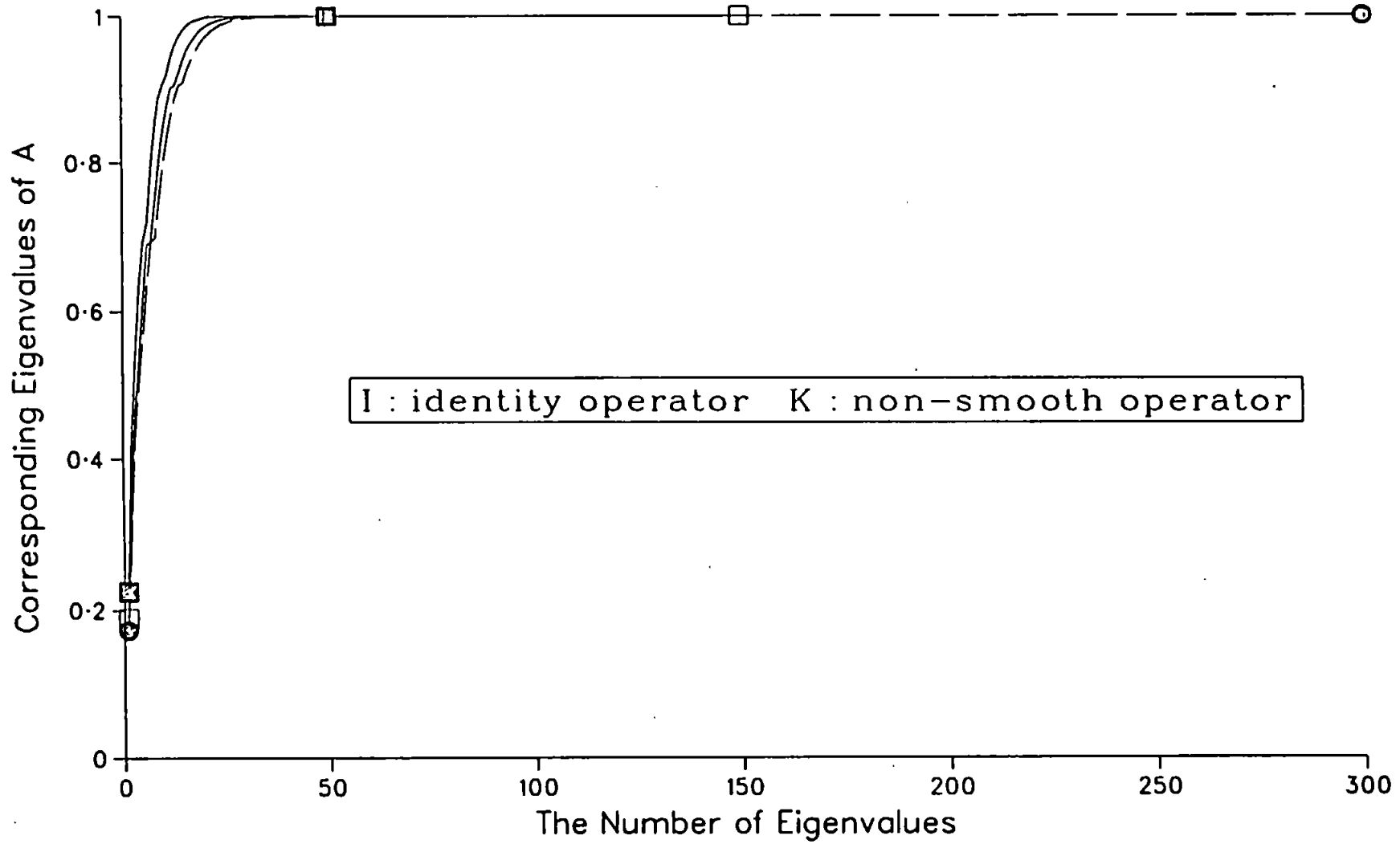


Fig.6.2 Approximate Eigenvalue Spectrum of $B = AA^*$ [constants, $q=1$]

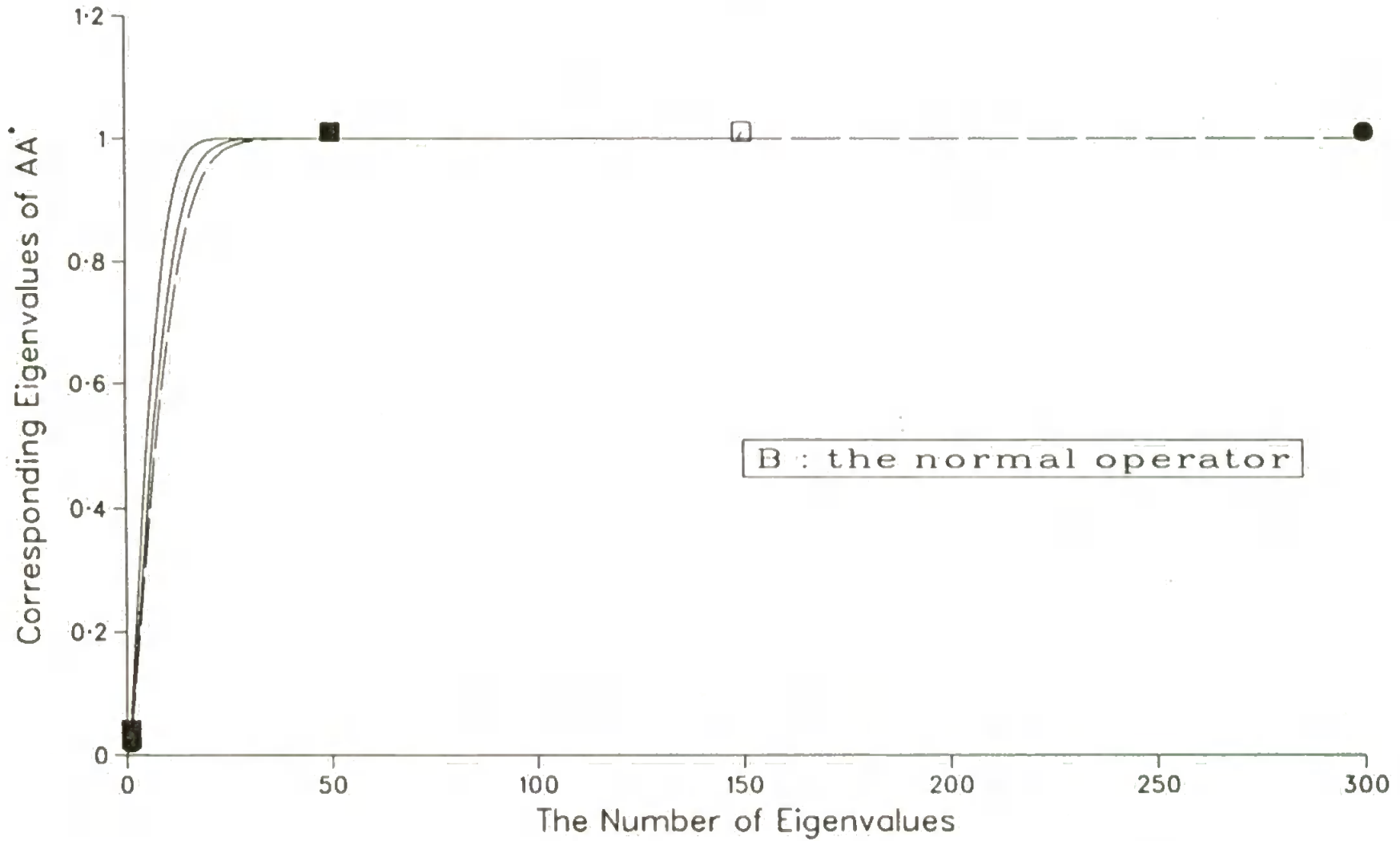


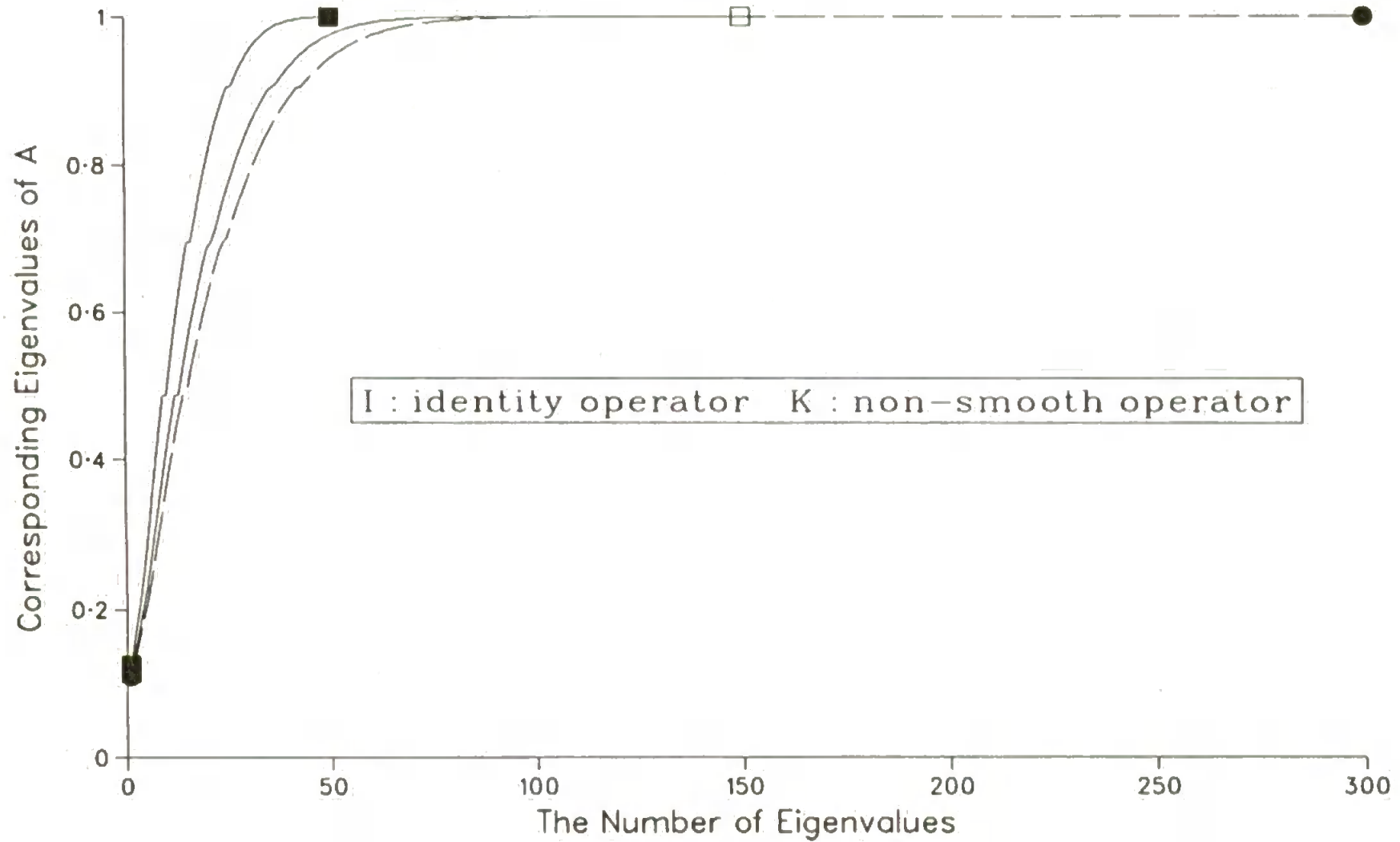
Fig.6.3 Approximate Eigenvalue Spectrum of $A = (I - K)$ [constants, $q=4$]

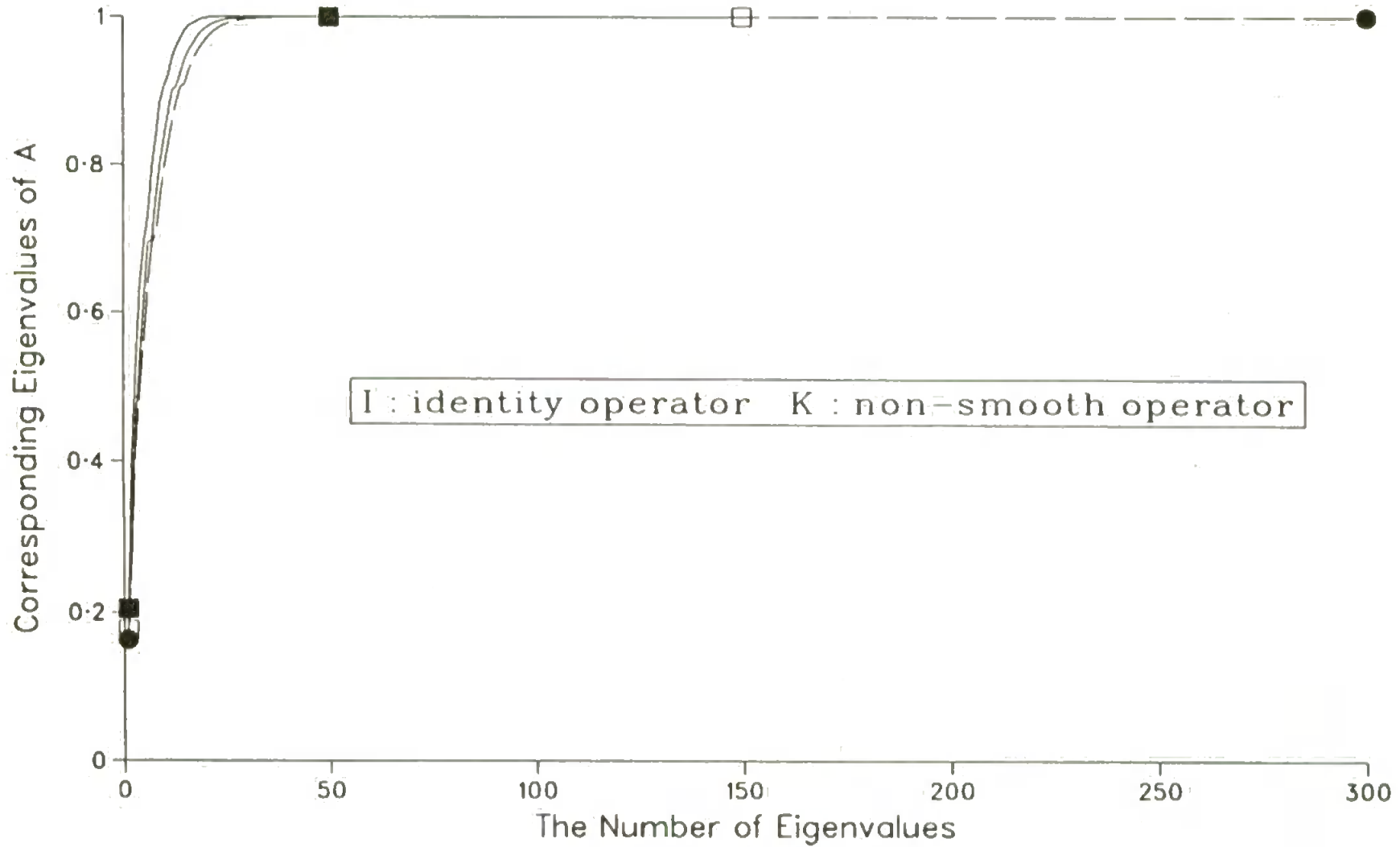
Fig.6.5 Approximate Eigenvalue Spectrum of $A = (I - K)$ [linears, $q=1$]

Fig.6.6 Approximate Eigenvalue Spectrum of $B = AA^*$ [linears, $q=1$]

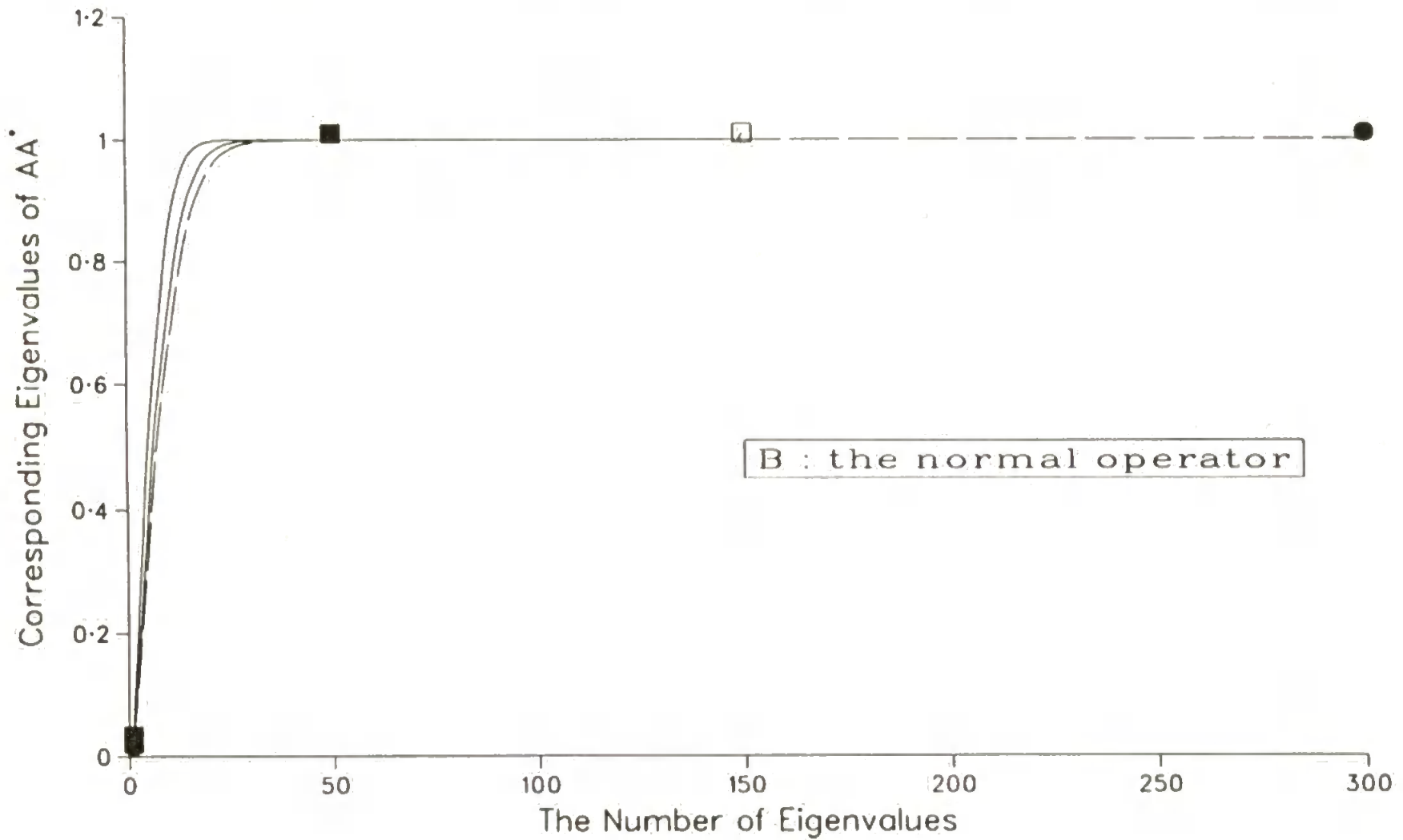


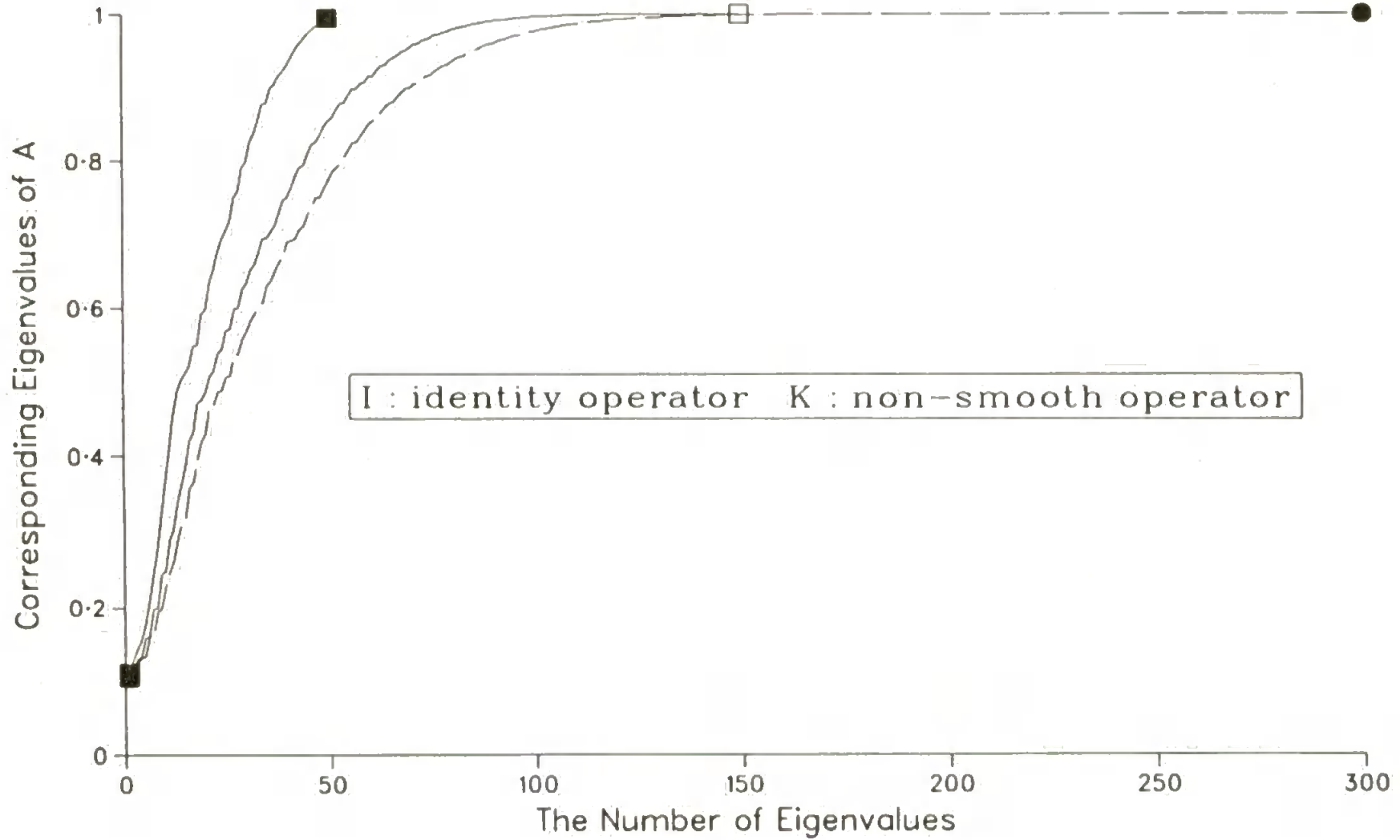
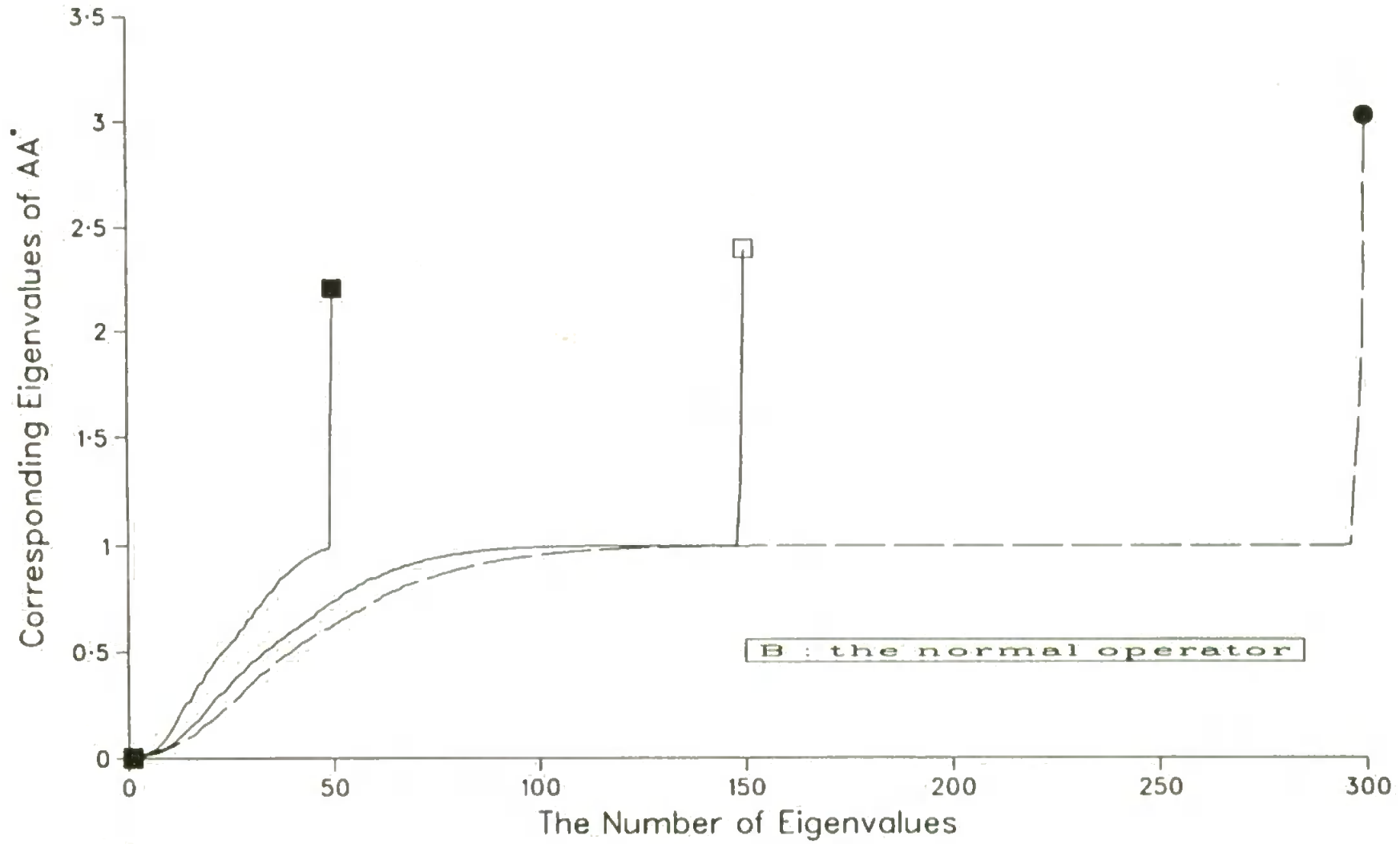
Fig.6.7 Approximate Eigenvalue Spectrum of $A = (I - K)$ [linears, $q=8$]

Fig.6.8 Approximate Eigenvalue Spectrum of $B = AA^*$ [linears, $q=8$]

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