A POSTERIORI ERROR ANALYSIS VIA DUALITY THEORY

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A POSTERIORI ERROR ANALYSIS VIA DUALITY THEORY

With Applications in Modeling and Numerical Approximations

by

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Dedicated to

DAQING HAN, SUZHEN QIN
HUIDI TANG
ELIZABETH, MICHAEL

Preface

This work provides a posteriori error analysis for mathematical idealizations in modeling boundary value problems, especially those arising in mechanical applications, and for numerical approximations of numerous nonlinear variational problems. An error estimate is called a posteriori if the computed solution is used in assessing its accuracy. A posteriori error estimation is central to measuring, controlling and minimizing errors in modeling and numerical approximations. In this book, the main mathematical tool for the developments of a posteriori error estimates is the duality theory of convex analysis, documented in the well-known book by Ekeland and Temam ([49]). The duality theory has been found useful in mathematical programming, mechanics, numerical analysis, etc.

The book is divided into six chapters. The first chapter reviews some basic notions and results from functional analysis, boundary value problems, elliptic variational inequalities, and finite element approximations. The most relevant part of the duality theory and convex analysis is briefly reviewed in Chapter 2. This brief review is sufficient for the applications of the duality theory in all the following chapters. In mathematical modeling of differential equation problems, usually assumptions are made on various data. Qualitatively, for many problems, it is known that the solution depends continuously on the problem data. Frequently though, it is desirable also to estimate or bound quantitatively the effect on the solutions of the problems caused by the adoption of the assumptions on the data. In Chapter 3, a posteriori error estimates are derived for the effect on the solutions of mathematical idealizations on the data of elliptic linear boundary value problems. In Chapter 4, a posteriori error estimates are given for linearization in a number of nonlinear boundary value problems. The last two chapters are devoted to a posteriori error analysis of numerical solutions. In Chapter 5, the regularization method and the Kačanov method are considered, both being useful in handling certain types of nonlinearity. In Chapter 6, a posteriori error estimates are derived and studied for finite element solutions of some elliptic variational inequalities.

This book is intended for researchers and graduate students in Applied and Computational Mathematics, and Engineering. Mathematical prerequisites include calculus, linear algebra, some exposures of differential equations, and concepts of normed spaces, Banach spaces and Hilbert spaces. In the theoretical development, some basic notions and results in functional analysis, duality thoery, weak formulations of boundary value problems, variational inequalities, and the finite element method are used. Brief reviews of these notions and results in the first two chapters provide background materials for a reader who lacks knowledge in these areas.

This work avoids giving the results in the most general, abstract form so that it is easier for the reader to understand more clearly the essential ideas involved. Many examples are included to show the usefulness of the derived error estimates.

In preparing this book, I have benefited from many individuals. I am grateful to Professor Ivo Babuška for introducing me the research topic and for providing valuable advice. Several of my collaborators (teachers, friends, and students) made contributions to various parts of the book, and I especially thank Dr. Viorel Bostan, Dr. Jiuhua Chen, Professor Hongci Huang, late Professor Søren Jensen, Professor B.D. Reddy. I express my gratitude to Professor Kendall Atkinson and Professor Mircea Sofonea for their constant support. I thank Professor D.Y. Gao and Professor R.W. Ogden for inviting me to make the contribution in their Kluwer book series on Advances in Mechanics and Mathematics (AMMA).

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Chapter 1

PRELIMINARIES

1.1. INTRODUCTION

Numerical simulation/scientific computation is now playing a more and more important role, and has become one of the three basic tools in science and technology, in addition to experimentation and theory. Numerical simulation provides a relatively inexpensive and efficient way to help understanding the physical world and advancing the technology.

A complete numerical analysis simulation session for a physical or engineering problem typically consists of several steps, described below. See Figure 1.1 for a description of the related flow chart, following [7].

First, the physical or engineering problem is brought to our attention. We want to predict and determine the response of the physical system to the external actions. To do this we need to establish a mathematical model for the problem. This is achieved by applying physical laws, material constitutive relations, and various experimental data such as the geometry of the system, densities of external forces. Most often, we obtain an initial-boundary or boundary value problem of differential equations or differential inequalities to describe the physical or engineering problem. We call this mathematical model the basic mathematical model, and identify it with the physical reality.

It is a highly idealized assumption that we can have a mathematical problem which exactly describes the physical problem. The available data, which usually come from experiments, for the basic mathematical formulation can not be obtained as accurate as one wishes. As a consequence, we solve a simplified, or idealized mathematical problem instead. The idealized or simplified problem is the mathematical model we use to study the physical problem.

The idealized mathematical model is usually still rather complicated and can be solved only by numerical methods. Popular methods to discretize initial-

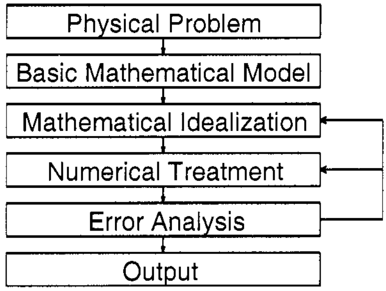

Figure 1.1. Numerical analysis of a physical problem

boundary or boundary value problems include the finite difference method and the finite element method. As a result of the discretization, we obtain a discrete system. The discrete system is then solved by some numerical method.

Once we have solved a discrete system, a natural question is: Can we use this solution? In other words, is this discrete solution sufficiently accurate for practical use? The reliability of a numerical solution of a physical or engineering problem depends on mathematical idealization of the physical problem and numerical treatment of the idealized mathematical problem. Various possibilities may arise and they demand our closer investigation. It is desirable to be able to estimate the errors associated with the steps described above. Standard topics in error analysis deal with the errors caused by discretization and solution of the discrete system. Fewer results are available for the estimation of errors in mathematical modelling. The error in mathematical modelling may be the most critical, however.

If both the mathematical idealization and the numerical solution of the idealized problem are reliable, various information for the real problem is drawn based on the numerical solution of the idealized problem. If a discrete solution is found to be not accurate enough, we need to trace the sources of the inaccuracy, and decide whether we need to compute a more accurate numerical solution of the mathematical model, or refine and numerically solve a new mathematical model.

There is a large amount of literature on numerical methods and their error analysis. Relatively few results are available in the literature for reliability analysis of mathematical idealizations, especially most desirably, certain good, practically useful quantitative assessments of the quality of solutions of idealized problems. Such quantitative assessments should be (hopefully) available once we have computed the solutions of idealized problems. One should not assume the quantitative knowledge of the solutions of basic mathematical problems for either exact descriptions of basic mathematical problems are usually not available in practice or, it is often too expensive to solve the basic mathematical problems. Some papers devoted to modeling error analysis or error analysis of mathematical idealizations include [30, 71, 72, 116, 118, 119, 120, 121, 128, 142].

An error estimate is called a posteriori if the computed solution is used in assessing its accuracy. A posteriori error estimation is central to measuring, controlling and minimizing errors in modeling and numerical approximations.

We now briefly describe the main features of the a posteriori error estimates to be derived and studied in this work. We let (P) stand for the basic mathematical model problem and use u for its solution, and let (P_0) be an idealized mathematical problem with the solution u_0, and (P_0^h) a numerical approximation of the idealized model with the solution u_0^h. Here, h represents a discretization parameter. The basic mathematical model (P) is usually difficult to solve, even numerically, and the simpler problem (P_0) is expected to be close to (P). We want to use the solution u_0 to bound the error $\|u - u_0\|$:

$$\|u - u_0\| \leq B(u_0),$$

where $B(u_0)$ is a quantity completely computable once u_0 and some information on the data of (P) are known. We also allow the case where the data for (P) are not completely given, and only some ranges of the data are available. In such a case, the data for (P_0) can be obtained through certain averaging process on the data for (P). Of course, to be able to derive a posteriori error estimates, we need to make assumptions on the structure of the problem (P). In this work, (P) is assumed to be a convex minimization problem; this allows the employment of the duality theory in convex analysis for deriving a posteriori error estimates. We will also use the numerical solution u_0^h of the problem (P_0^h) to bound the error $\|u_0 - u_0^h\|$. A posteriori estimation of the discretization error $(u_0 - u_0^h)$ has been a popular research topic since late 1970's (see the description in Chapter 6). Many of the a posteriori error estimates for the numerical solutions of differential equation problems can be derived via the duality theory. In Chapter 6, we focus on the a posteriori error analysis for finite element solutions of elliptic variational inequalities of the second kind. We will see there that the duality approach provides a general framework, leading to various a posteriori error estimators.

In this work, errors are measured in terms of energy norms or energy-like norms. The salient features of the a posteriori error estimates presented in this work are:

1 The error estimates are rigorous in the sense that the error bounds are always satisfied. In this sense, when we say error estimates, most often we mean error bounds. We use the phrases "error estimates" and "error bounds" interchangeably.

2 The error bounds are determined by the solutions of the idealized mathematical models or the numerical solutions of the given problems. There is no need to solve related dual problems.

3 All the error bounds, except those presented in Chapter 6 on the finite element approximations of variational inequalities, are completely computable in the sense that there are no unknown constants. In the literature, most a posteriori error estimates on numerical solutions of partial differential equations problems involve such theoretical unknown constants and their values are selected based on a few numerical examples (e.g., [50]).

4 Efficiency of the error estimates is demonstrated through numerous examples and theoretical analysis.

Recently, goal-oriented or object-oriented error estimates have been developed to calculate error bounds of global or local quantities of interest, such as the error of stress or strain in a critical region, using a dual-weighted residual technique. The procedure of the technique can be described as follows. Consider a boundary value problem and suppose the purpose of the computation is the value of a functional of the solution. The boundary value problem is solved numerically, typically by the finite element method. The functional of the numerical solution is then computed. To bound the error involved in the functional value, a dual problem is introduced related to the functional and the boundary value problem, and is numerically solved. Then the error in the computed functional value is expressed in terms of the numerical solution of the dual problem together with some residual quantities, which is then localized and split into contributions related to the modeling error and discretization error. The survey papers [19, 62] provide detailed accounts of this technique. Note that the use of solutions of the dual problems may imply a possibly dramatic increase in the computational effort. In this work, dual problems will play a central role in the derivation of error estimators, but the error bounds do not involve solutions of the dual problems.

The organization of the book is the following. In the remaining part of this first chapter, we will briefly review some basic notions and results from functional analysis, function spaces, weak formulation of boundary value problems, and the finite element method. In Chapter 2, we review some basic material from convex analysis and the duality theory, that plays the central role in this book for a posteriori error analysis. In Chapter 3, we employ the duality theory to derive a posteriori error estimates for mathematical idealizations in linear boundary value problems, paying particular attention to the situation with nonsmooth domains. The idealizations can occur in the coefficients of the differential equations, the right-hand sides, boundary value conditions, and the domain. In Chapter 4, we perform a posteriori error analysis for the effect of linearization in several nonlinear problems. In Chapter 5, we apply the duality theory to derive a posteriori error estimates for some numerical procedures in solving nonlinear boundary value problems, including the regularization method for problems involving non-differentiable terms, Kačanov iteration methods and linearizations. Finally, in Chapter 6, we derive a posteriori error estimates for finite element solutions of elliptic variational inequalities of the second kind. The error estimates that can be derived via the duality theory include some of the well-known a posteriori error estimates found in the finite element literature for solving elliptic differential equations.

1.2. SOME BASIC NOTIONS FROM FUNCTIONAL ANALYSIS

We assume the reader is familiar with such basic notions as linear spaces, norms, inner products, Banach spaces, and Hilbert spaces. Details on these and the material to be reviewed in the following can be found in any standard textbook on functional analysis, e.g., [45, 48], or in a concise form, [6].

In this work, the general theory will be developed for domains in the space $\mathbb{R}^d$ of the d-dimensional vectors of the form $\boldsymbol{x} = (x_1, \dots, x_d)^T$, $x_i \in \mathbb{R}$. Recall that a domain $\Omega \subset \mathbb{R}^d$ is an open, connected, bounded set in $\mathbb{R}^d$. For $p \in [1, \infty]$, we have the following norms in $\mathbb{R}^d$:

$$|\boldsymbol{x}|_p = \begin{cases} \left(\sum\limits_{i=1}^{d} |x_i|^p\right)^{1/p} & 1 \le p < \infty, \\ \max\limits_{i} |x_i| & p = \infty. \end{cases}$$

When $\mathbb{R}^d$ is viewed as a normed space, implicitly we understand the norm to be the Euclidean norm $|\cdot| \equiv |\cdot|_2$, unless otherwise stated. The Euclidean norm is induced by the canonical inner product in $\mathbb{R}^d$:

$$|\boldsymbol{x}| = (\boldsymbol{x}, \boldsymbol{x})^{1/2}, \quad (\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{d} x_i y_i \quad \forall\, \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d.$$

The summation convention over a repeated index will be adopted. As an example, for the canonical inner product in $\mathbb{R}^d$, we write $(\boldsymbol{x}, \boldsymbol{y}) = x_i y_i$.

The symbol $\mathbb{S}^d$ stands for the space of second order symmetric tensors on $\mathbb{R}^d$ or, equivalently, the space of symmetric matrices of order d. The inner product and corresponding norm on $\mathbb{S}^d$ are

$$\boldsymbol{\sigma} \cdot \boldsymbol{\tau} = \sigma_{ij} \tau_{ij}, \quad \|\boldsymbol{\tau}\| = (\boldsymbol{\tau} \cdot \boldsymbol{\tau})^{1/2} \quad \forall\, \boldsymbol{\sigma}, \boldsymbol{\tau} \in \mathbb{S}^d.$$

For a normed space V, we use V^* to denote its *dual space*, i.e., the space of all the continuous linear functionals on V. The duality pairing between V^* and V is usually denoted by $\ell(v)$ or $\langle v^*, v \rangle$ for $\ell, v^* \in V^*$ and $v \in V$. We can then introduce different types of convergence.

DEFINITION 1.1 *Let V be a normed space, V^* its dual space. A sequence $\{u_n\} \subset V$* converges *or* converges strongly *to $u \in V$, written $u_n \to u$ as $n \to \infty$, if*

$$\lim_{n\to\infty} \|u - u_n\| = 0.$$

The sequence $\{u_n\}$ converges weakly *to $u \in V$, written $u_n \rightharpoonup u$ as $n \to \infty$, if*

$$\ell(u_n) \to \ell(u) \quad \text{as } n \to \infty, \quad \forall\, \ell \in V^*.$$

We will use the following property of a weakly convergent sequence:

$$u_n \rightharpoonup u \quad \Longrightarrow \quad \|u\| \le \liminf_{n\to\infty} \|u_n\|. \tag{1.1}$$

The dual space of a normed space is always complete, i.e. always a Banach space. Over a finite dimensional space, it is a well-known result that any bounded sequence contains a convergent subsequence. This property does not carry over to infinite dimensional spaces. For example, the sequence $\{\sin j\pi x\}_{j\ge 1}$ is a bounded sequence in $L^2(0,1)$, but none of its subsequences converges. In many applications of the functional analytic approach, one needs the property that a bounded sequence contains a subsequence that converges in some sense. Reflexive Banach spaces enjoy this kind of desirable property. A space V is said to be *reflexive* if $(V^*)^*$ can be identified with V. A reflexive space must be complete and is hence a Banach space. We have the following important property of a reflexive space.

THEOREM 1.2 *If V is a reflexive Banach space, then any bounded sequence in V has a weakly convergent subsequence.*

We will see examples of reflexive Banach spaces in Section 1.3.

For an inner product, there is an important property called the Cauchy–Schwarz inequality:

$$|(u,v)| \le \sqrt{(u,u)\,(v,v)} \quad \forall\, u, v \in V,$$

with the equality holding iff u and v being linearly dependent. We recall an important property of a Hilbert space.

THEOREM 1.3 (*Riesz representation theorem*) *Let V be a Hilbert space, $\ell \in V^*$. Then there is a unique $u \in V$ for which*

$$\ell(v) = (v,u) \quad \forall\, v \in V.$$

In addition,

$$\|\ell\| = \|u\|_V.$$

Thus, the dual space of a Hilbert space can be identified with itself, and any Hilbert space is reflexive.

1.3. FUNCTION SPACES

We will use the multi-index notation for partial derivatives. An ordered collection of d non-negative integers, $\alpha = (\alpha_1, \ldots, \alpha_d)$, is called a multi-index. The quantity $|\alpha| = \sum_{i=1}^{d} \alpha_i$ is said to be the length of α. If v is an m-times differentiable function, then for any α with $|\alpha| \le m$,

$$D^\alpha v(\boldsymbol{x}) = \frac{\partial^{|\alpha|} v(\boldsymbol{x})}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}$$

is the αth order partial derivative. For lower order partial derivatives, there are other notations in common use; e.g., the partial derivative $\partial v/\partial x_i$ is also written as $\partial_{x_i} v$, or $\partial_i v$, or $v_{,x_i}$, or $v_{,i}$.

1.3.1 CONTINUOUS FUNCTION SPACES

The notation $C(\overline{\Omega})$ is used for the space of functions continuous on $\overline{\Omega}$. It is a Banach space with the norm

$$\|v\|_{C(\overline{\Omega})} = \sup\{|v(\boldsymbol{x})| : \boldsymbol{x} \in \Omega\} \equiv \max\{|v(\boldsymbol{x})| : \boldsymbol{x} \in \overline{\Omega}\}.$$

More generally, for a non-negative integer m, we define

$$C^m(\overline{\Omega}) = \{v \in C(\overline{\Omega}) : D^\alpha v \in C(\overline{\Omega}) \text{ for } |\alpha| \le m\},$$

which is a Banach space with the norm

$$\|v\|_{C^m(\overline{\Omega})} = \sum_{|\alpha| \le m} \|D^\alpha v\|_{C(\overline{\Omega})}.$$

We also set

$$C^\infty(\overline{\Omega}) = \cap_{m=0}^{\infty} C^m(\overline{\Omega}) \equiv \{v \in C(\overline{\Omega}) : v \in C^m(\overline{\Omega})\ \forall\, m = 0, 1, \ldots\}.$$

Given a function v on Ω, its support is defined to be

$$\operatorname{supp} v = \overline{\{\boldsymbol{x} \in \Omega : v(\boldsymbol{x}) \ne 0\}}.$$

Here a bar over a set stands for the closure of the set. We say that v has a *compact support* if $\operatorname{supp} v$ is a proper subset of Ω: $\operatorname{supp} v \subset\subset \Omega$. Thus, if v has a compact support, then there is a strip about the boundary $\partial\Omega$ such that v is zero on the intersection of the strip and the domain. Later on, we will use the space

$$C_0^\infty(\Omega) = \{v \in C^\infty(\Omega) : \operatorname{supp} v \subset\subset \Omega\}.$$

Hölder spaces. A function v defined on Ω is said to be *Lipschitz continuous* if for some constant c,

$$|v(\boldsymbol{x}) - v(\boldsymbol{y})| \le c\,|\boldsymbol{x} - \boldsymbol{y}| \quad \forall\, \boldsymbol{x}, \boldsymbol{y} \in \Omega.$$

The smallest possible constant in the above inequality is called the Lipschitz constant of v, and is denoted by $\mathrm{Lip}(v)$. More generally, the function v is said to be Hölder continuous with exponent $\beta \in (0,1]$ if for some constant c,

$$|v(\boldsymbol{x}) - v(\boldsymbol{y})| \leq c\,|\boldsymbol{x} - \boldsymbol{y}|^{\beta} \quad \forall\, \boldsymbol{x}, \boldsymbol{y} \in \Omega.$$

The Hölder space $C^{0,\beta}(\overline{\Omega})$ is defined to be the subspace of $C(\overline{\Omega})$ which consists of functions Hölder continuous with the exponent β. With the norm

$$\|v\|_{C^{0,\beta}(\overline{\Omega})} = \|v\|_{C(\overline{\Omega})} + \sup\left\{\frac{|v(\boldsymbol{x}) - v(\boldsymbol{y})|}{|\boldsymbol{x} - \boldsymbol{y}|^{\beta}} : \boldsymbol{x}, \boldsymbol{y} \in \Omega,\ \boldsymbol{x} \neq \boldsymbol{y}\right\},$$

the space $C^{0,\beta}(\overline{\Omega})$ becomes a Banach space.

For a nonnegative integer m and $\beta \in (0,1]$, we similarly define the Hölder space

$$C^{m,\beta}(\overline{\Omega}) = \left\{v \in C^{m}(\overline{\Omega}) : D^{\alpha}v \in C^{0,\beta}(\overline{\Omega}) \text{ for all } \alpha \text{ with } |\alpha| = m\right\};$$

this is a Banach space with the norm

$$\begin{aligned}\|v\|_{C^{m,\beta}(\overline{\Omega})} &= \|v\|_{C^{m}(\overline{\Omega})} \\ &\quad + \sum_{|\alpha|=m} \sup\left\{\frac{|D^{\alpha}v(\boldsymbol{x}) - D^{\alpha}v(\boldsymbol{y})|}{|\boldsymbol{x} - \boldsymbol{y}|^{\beta}} : \boldsymbol{x}, \boldsymbol{y} \in \Omega,\ \boldsymbol{x} \neq \boldsymbol{y}\right\}.\end{aligned}$$

1.3.2 LEBESGUE SPACES

In the study of Lebesgue spaces, we identify functions which are equal a.e. on Ω. For $p \in [1, \infty)$, $L^{p}(\Omega)$ is the linear space of measurable functions $v : \Omega \to \mathbb{R}$ such that

$$\|v\|_{L^{p}(\Omega)} = \left\{\int_{\Omega} |v(\boldsymbol{x})|^{p} dx\right\}^{1/p} < \infty. \tag{1.2}$$

The space $L^{\infty}(\Omega)$ consists of all essentially bounded measurable functions $v : \Omega \to \mathbb{R}$ such that

$$\|v\|_{L^{\infty}(\Omega)} = \inf_{\mathrm{meas}(\Omega')=0} \ \sup_{\boldsymbol{x} \in \Omega \setminus \Omega'} |v(\boldsymbol{x})| < \infty. \tag{1.3}$$

For a measurable function v defined on Ω, if $v \in L^{p}(\Omega')$ for any $\Omega' \subset\subset \Omega$, then we say v is locally in $L^{p}(\Omega)$ and write $v \in L^{p}_{\mathrm{loc}}(\Omega)$. We use $\mathrm{meas}(\Omega)$ for the Lebesgue measure of Ω. For $d = 3$, $\mathrm{meas}(\Omega)$ is the volume of Ω, and for $d = 2$, $\mathrm{meas}(\Omega)$ is the area of Ω.

Some basic properties of the L^{p} spaces are summarized in the following theorem.

THEOREM 1.4 *Let Ω be an open bounded set in $\mathbb{R}^d$.*
(a) *For $p \in [1, \infty]$, $L^p(\Omega)$ is a Banach space with the norm defined in* (1.2) *or* (1.3).
(b) *For $p \in [1, \infty]$, every Cauchy sequence in $L^p(\Omega)$ has a subsequence which converges pointwise a.e. on Ω.*
(c) *If $1 \le p \le q \le \infty$, then $L^q(\Omega) \subset L^p(\Omega)$,*

$$\|v\|_{L^p(\Omega)} \le \text{meas}(\Omega)^{1/p-1/q} \|v\|_{L^q(\Omega)} \quad \forall\, v \in L^q(\Omega),$$

and

$$\|v\|_{L^\infty(\Omega)} = \lim_{p \to \infty} \|v\|_{L^p(\Omega)} \quad \forall\, v \in L^\infty(\Omega).$$

(d) *If $1 \le p \le r \le q \le \infty$ and we choose $\theta \in [0, 1]$ such that $1/r = \theta/p + (1-\theta)/q$, then*

$$\|v\|_{L^r(\Omega)} \le \|v\|^{\theta}_{L^p(\Omega)} \|v\|^{1-\theta}_{L^q(\Omega)} \quad \forall\, v \in L^q(\Omega).$$

(e) *For $1 \le p < \infty$, $(L^p(\Omega))^* = L^{p^*}(\Omega)$. Hence for $p \in (1, \infty)$, the space $L^p(\Omega)$ is reflexive.*

1.3.3 SOBOLEV SPACES

Sobolev spaces are defined based on the concept of weak derivatives.

DEFINITION 1.5 *Let Ω be a nonempty open set in $\mathbb{R}^d$, $v, w \in L^1_{\text{loc}}(\Omega)$. Then w is called an α^{th}* weak derivative *of v if*

$$\int_\Omega v(\boldsymbol{x})\, D^\alpha \phi(\boldsymbol{x})\, dx = (-1)^{|\alpha|} \int_\Omega w(\boldsymbol{x})\, \phi(\boldsymbol{x})\, dx \quad \forall\, \phi \in C_0^\infty(\Omega).$$

It follows from the definition that a weak derivative, if it exists, is unique up to a set of measure zero. Another direct consequence of Definition 1.5 is that if a function v has a continuous α^{th} derivative $D^\alpha v$ in the classical sense, then $D^\alpha v$ is also the α^{th} weak derivative of v. Thus we see that the notion of a weak derivative is indeed an extension of the classical derivative. For this reason, we will use the symbol $D^\alpha v$ for the α^{th} weak derivative of v.

Let k be a nonnegative integer, $p \in [1, \infty]$.

DEFINITION 1.6 *The Sobolev space $W^{k,p}(\Omega)$ is the set of all the functions $v \in L^1_{\text{loc}}(\Omega)$ such that for each multi-index α with $|\alpha| \le k$, the α^{th} weak derivative $D^\alpha v$ exists and $D^\alpha v \in L^p(\Omega)$. The norm in the space $W^{k,p}(\Omega)$ is defined by the following:*

$$\|v\|_{W^{k,p}(\Omega)} = \begin{cases} \left(\sum_{|\alpha| \le k} \|D^\alpha v\|^p_{L^p(\Omega)} \right)^{1/p} & \text{if } 1 \le p < \infty, \\ \max_{|\alpha| \le k} \|D^\alpha v\|_{L^\infty(\Omega)} & \text{if } p = \infty. \end{cases}$$

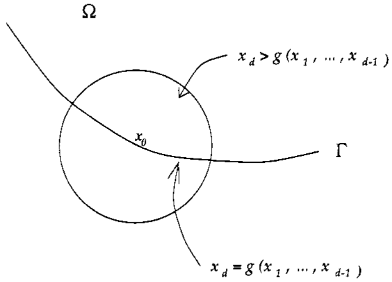

Figure 1.2. Smoothness of the boundary

When $p = 2$, we write $H^k(\Omega) \equiv W^{k,2}(\Omega)$.

We will mainly use Sobolev spaces $W^{k,p}(\Omega)$ when Ω is a domain in $\mathbb{R}^d$.

Usually we use simpler notation $\|\cdot\|_{k,p,\Omega}$ to denote the norm $\|\cdot\|_{W^{k,p}(\Omega)}$, and $\|\cdot\|_{k,\Omega}$ for the norm $\|\cdot\|_{H^k(\Omega)}$. The Sobolev space $W^{k,p}(\Omega)$ is a Banach space, and $H^k(\Omega)$ is a Hilbert space with the inner product

$$(u, v)_{k,\Omega} = \int_\Omega \sum_{|\alpha| \le k} D^\alpha u(\boldsymbol{x})\, D^\alpha v(\boldsymbol{x})\, dx, \quad u, v \in H^k(\Omega).$$

Next we list several important properties of Sobolev spaces. Some properties require a certain degree of smoothness of the boundary Γ of the domain Ω.

DEFINITION 1.7 *Let Ω be open bounded in $\mathbb{R}^d$, and let V denote a function space on $\mathbb{R}^{d-1}$. We say $\partial\Omega$ is of class V if for each point $\boldsymbol{x}_0 \in \partial\Omega$, there exist an $r > 0$ and a function $g \in V$ such that upon relabelling the coordinate axes if necessary, we have*

$$\Omega \cap B(\boldsymbol{x}_0, r) = \{\boldsymbol{x} \in B(\boldsymbol{x}_0, r) : x_d > g(x_1, \cdots, x_{d-1})\}.$$

Here, $B(\boldsymbol{x}_0, r)$ denotes the ball centered at $\boldsymbol{x}_0$ with radius r. See Figure 1.2.

In particular, when V consists of Lipschitz continuous functions, we say Ω is a Lipschitz domain. When V consists of C^k functions, we say Ω is a C^k domain.

Since $\partial\Omega$ is a compact set in $\mathbb{R}^d$, we can actually find a finite number of points $\{\boldsymbol{x}_i\}_{i=1}^I$ on the boundary so that for some positive numbers $\{r_i\}_{i=1}^I$ and functions $\{g_i\}_{i=1}^I \subset V$,

$$\Omega \cap B(\boldsymbol{x}_i, r_i) = \{\boldsymbol{x} \in B(\boldsymbol{x}_i, r_i) : x_d > g_i(x_1, \cdots, x_{d-1})\}$$

upon relabelling the coordinate axes if necessary, and

$$\Gamma \subset \cup_{i=1}^I B(\boldsymbol{x}_i, r_i).$$

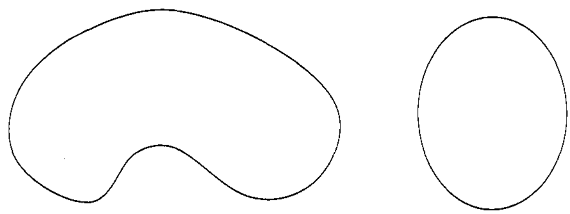

Figure 1.3. Smooth domains

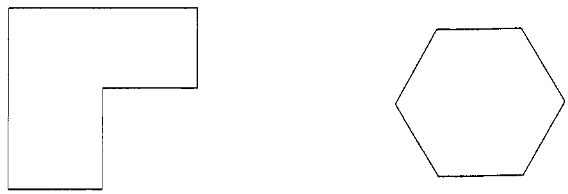

Figure 1.4. Lipschitz domains

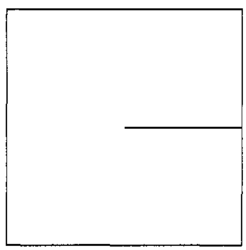

Figure 1.5. A crack domain

Throughout this work, we will assume Ω is Lipschitz continuous, unless stated explicitly otherwise. We observe that in engineering applications, most domains are Lipschitz continuous (Figures 1.3 and 1.4). A well-known non-Lipschitz domain is one with cracks (Figure 1.5).

Approximation by smooth functions. Equalities and inequalities involving Sobolev functions are usually proved first for smooth functions followed by a density argument. A theoretical basis for this technique is results on density of smooth functions in Sobolev spaces.

THEOREM 1.8 *Assume Ω is a Lipschitz domain, $1 \le p < \infty$. Then for any $v \in W^{k,p}(\Omega)$, there exists a sequence $\{v_n\} \subset C^\infty(\overline{\Omega})$ such that*

$$\|v_n - v\|_{k,p,\Omega} \to 0 \quad as\ n \to \infty.$$

Proof of this density theorem can be found, e.g., in [51].

DEFINITION 1.9 *We define $W_0^{k,p}(\Omega)$ as the closure of $C_0^\infty(\Omega)$ in $W^{k,p}(\Omega)$. When $p = 2$, we denote $H_0^k(\Omega) \equiv W_0^{k,2}(\Omega)$.*

From Definition 1.9, we see that we always have the denseness of the smooth function space $C_0^\infty(\Omega)$ in $W_0^{k,p}(\Omega)$. We interpret $W_0^{k,p}(\Omega)$ to be the space of all the functions v in $W^{k,p}(\Omega)$ with the "property" that

$$D^\alpha v(\boldsymbol{x}) = 0 \quad \text{on } \partial\Omega,\ \forall\, \alpha \text{ with } |\alpha| \le k-1.$$

The meaning of this statement will be made clear later after the trace theorems are presented.

Traces. Notice that Sobolev spaces are defined through Lebesgue spaces. Hence Sobolev functions are uniquely defined only a.e. in Ω. Since the boundary $\partial\Omega$ has measure zero in $\mathbb{R}^d$, it seems the boundary value of a Sobolev function is not well-defined. Nevertheless it is possible to define the trace of a Sobolev function on the boundary in such a way that for a Sobolev function continuous up to the boundary, its trace coincides with its boundary value.

THEOREM 1.10 *Assume Ω is a Lipschitz domain in $\mathbb{R}^d$, $1 \le p < \infty$. Then there exists a linear operator $\gamma : W^{1,p}(\Omega) \to L^p(\partial\Omega)$ such that*
(a) *$\gamma v = v|_{\partial\Omega}$ if $v \in W^{1,p}(\Omega) \cap C(\overline{\Omega})$.*
(b) *For some constant $c > 0$, $\|\gamma v\|_{L^p(\partial\Omega)} \le c\,\|v\|_{W^{1,p}(\Omega)}$ $\forall\, v \in W^{1,p}(\Omega)$.*
(c) *The mapping $\gamma : W^{1,p}(\Omega) \to L^p(\partial\Omega)$ is compact; i.e., for any bounded sequence $\{v_n\}$ in $W^{1,p}(\Omega)$, there is a subsequence $\{v_{n'}\} \subset \{v_n\}$ such that $\{\gamma v_{n'}\}$ is convergent in $L^p(\partial\Omega)$.*

In Theorem 1.10, the Lebesgue spaces on the boundary, $L^p(\partial\Omega)$, are used. A precise definition of these spaces can be found in [101, Section 6.3].

The operator γ is called the trace operator, and with property (a) we can view γv as the the generalized boundary value of v. Property (b) states that the mapping γ is continuous from $W^{1,p}(\Omega)$ to $L^p(\partial\Omega)$, whereas property (c) further states that actually the mapping γ is compact from $W^{1,p}(\Omega)$ to $L^p(\partial\Omega)$. The trace operator is neither an injection nor a surjection from $W^{1,p}(\Omega)$ to $L^p(\partial\Omega)$. The range $\gamma(W^{1,p}(\Omega))$ is actually a space smaller than $L^p(\partial\Omega)$, that is denoted by $W^{1-1/p,p}(\partial\Omega)$, an example of a fractional order Sobolev space. This is a Banach space with the norm

$$\|g\|_{W^{1-1/p,p}(\partial\Omega)} = \inf_{\substack{v \in W^{1,p}(\Omega) \\ \gamma v = g}} \|v\|_{W^{1,p}(\Omega)}.$$

We will frequently use the space $H^{1/2}(\partial\Omega) \equiv \gamma(H^1(\Omega))$. In the future to simplify the notation, for a function $v \in W^{1,p}(\Omega)$, we will denote its trace on the boundary also by v. The trace operator is also continuous from

$W^{1,p}(\Omega)$ to $L^q(\Omega)$ for q in certain range. One such example is: for $d = 2$, $\gamma \in \mathcal{L}(H^1(\Omega), H^q(\partial\Omega))$ for any $q \in [1, \infty)$, and for some constant $c = c(\Omega, q)$, we have the inequality

$$\|v\|_{L^q(\partial\Omega)} \le c\,\|v\|_{H^1(\Omega)} \quad \forall\, v \in H^1(\Omega). \tag{1.4}$$

With the notion of the trace of $W^{1,p}(\Omega)$ functions, we have

$$W_0^{1,p}(\Omega) = \{v \in W^{1,p}(\Omega) : v = 0 \text{ on } \partial\Omega\}.$$

Here, the condition "$v = 0$ on $\partial\Omega$" is understood as that the trace of v is a zero function on $\partial\Omega$. This condition can be equivalently stated as "$v = 0$ a.e. on $\partial\Omega$". The particular case $p = 2$ leads to the Hilbert space

$$H_0^1(\Omega) = \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega\}.$$

Its dual space is usually denoted as $H^{-1}(\Omega)$.

In some occasions, we will need to use the first derivatives (e.g., the normal derivative) on the boundary. Let $\boldsymbol{\nu} = (\nu_1, \cdots, \nu_d)^T$ denote the outward unit normal to the boundary Γ of Ω. Since $\partial\Omega$ is Lipschitz continuous, $\boldsymbol{\nu}$ exists a.e. on $\partial\Omega$. For a function $v \in H^2(\Omega)$, its first derivatives $v_{x_i} \in H^1(\Omega)$. By Theorem 1.10, it is meaningful to write their traces $v_{x_i} \in L^2(\partial\Omega)$. We can then define the normal derivative

$$\frac{\partial v}{\partial \nu} = \nu_i \frac{\partial v}{\partial x_i}$$

and we have the integration by parts formula

$$\int_\Omega (\Delta u\, v + \nabla u \cdot \nabla v)\, dx = \int_{\partial\Omega} \frac{\partial u}{\partial \nu}\, v\, ds \quad \forall\, u \in H^2(\Omega),\ v \in H^1(\Omega).$$

This formula is first proved for $u, v \in C^\infty(\overline{\Omega})$, and is then extended to $u \in H^2(\Omega)$ and $v \in H^1(\Omega)$ by applying the density result Theorem 1.8.

For boundary value problems of higher-order partial differential equations, we need to use the traces of partial derivatives on the boundary. Such results can be found in, e.g., [67].

Sobolev embedding theorems. Sobolev embedding theorems are important, especially in analyzing the regularity of a weak solution of a boundary value problem.

DEFINITION 1.11 *Let V and W be two Banach spaces with $V \subset W$. We say the space V is continuously embedded in W and write $V \hookrightarrow W$ if there exists a constant $c > 0$ such that*

$$\|v\|_W \le c\,\|v\|_V \quad \forall\, v \in V. \tag{1.5}$$

We say the space V is compactly embedded in W and write $V \hookrightarrow\hookrightarrow W$, if (1.5) *holds and each bounded sequence in V has a convergent subsequence in W.*

If $V \hookrightarrow W$, the functions in V are smoother than the rest of the functions in W. Proofs of most parts of the following two theorems can be found in [51]. The first theorem is on embedding of Sobolev spaces, and the second on compact embedding. These theorems are given in a form more general than what is needed later in this work. For any $t \in \mathbb{R}$, we denote $[t]$ the largest integer less than or equal to t.

THEOREM 1.12 *Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain. Then the following statements are valid.*
(a) *If $k < d/p$, then $W^{k,p}(\Omega) \hookrightarrow L^q(\Omega)$ for any $q \le p'$, where $1/p' = 1/p - k/d$.*
(b) *If $k = d/p$, then $W^{k,p}(\Omega) \hookrightarrow L^q(\Omega)$ for any $q < \infty$.*
(c) *If $k > d/p$, then*

$$W^{k,p}(\Omega) \hookrightarrow C^{k-[d/p]-1,\beta}(\Omega),$$

where

$$\beta = \begin{cases} [d/p] + 1 - d/p & \textit{if } d/p \neq \textit{integer}, \\ \textit{any positive number} < 1 & \textit{if } d/p = \textit{integer}. \end{cases}$$

THEOREM 1.13 *Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain. Then the following statements are valid.*
(a) *If $k < d/p$, then $W^{k,p}(\Omega) \hookrightarrow\hookrightarrow L^q(\Omega)$ for any $q < p'$, where $1/p' = 1/p - k/d$.*
(b) *If $k = d/p$, then $W^{k,p}(\Omega) \hookrightarrow\hookrightarrow L^q(\Omega)$ for any $q < \infty$.*
(c) *If $k > d/p$, then*

$$W^{k,p}(\Omega) \hookrightarrow\hookrightarrow C^{k-[d/p]-1,\beta}(\Omega),$$

where $\beta \in [0, [d/p] + 1 - d/p)$.

Equivalent norms. Associated with any vector space, one can define infinitely many different norms. A well-known result in analysis states that over a finite dimensional space, any two norms are equivalent, i.e., if $\|\cdot\|^{(1)}$ and $\|\cdot\|^{(2)}$ are two norms on a finite dimensional space V, then there exist two constants $0 < c_1 \le c_2 < \infty$ such that

$$c_1 \|v\|^{(2)} \le \|v\|^{(1)} \le c_2 \|v\|^{(2)} \quad \forall v \in V.$$

Thus, in a finite dimensional space, different norms lead to the same convergence property. For an infinite dimensional space, however, not any two norms are equivalent. For example, over the space $C[0,1]$, the norm $\|\cdot\|_{C[0,1]}$ is stronger than $\|\cdot\|_{L^1(0,1)}$: A sequence converging with respect to the norm $\|\cdot\|_{C[0,1]}$ converges also with respect to the norm $\|\cdot\|_{L^1(0,1)}$, whereas it is easy to construct examples of function sequences converging with respect to $\|\cdot\|_{L^1(0,1)}$ but not with respect to $\|\cdot\|_{C[0,1]}$ (cf. [6, Example 1.2.13]). In some applications, it is convenient to use a different norm that is equivalent to the canonical norm of a given space. The next result can be used to generate various equivalent norms on Sobolev spaces. Over the Sobolev space $W^{k,p}(\Omega)$, $|v|_{k,p,\Omega}$ is the seminorm defined by

$$|v|_{k,p,\Omega} = \left(\int_\Omega \sum_{|\alpha|=k} |D^\alpha v(\boldsymbol{x})|^p \, dx \right)^{1/p}.$$

It can be shown that if Ω is connected and $|v|_{k,p,\Omega} = 0$, then v is a polynomial of degree less than or equal to $k-1$.

THEOREM 1.14 *Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain, $k \geq 1$, $1 \leq p < \infty$. Assume $f_j : W^{k,p}(\Omega) \to \mathbb{R}$, $1 \leq j \leq J$, are seminorms on $W^{k,p}(\Omega)$ satisfying two conditions:*

(H$_1$) $0 \leq f_j(v) \leq c\,\|v\|_{k,p,\Omega}$ $\forall\, v \in W^{k,p}(\Omega)$, $1 \leq j \leq J$.
(H$_2$) *If v is a polynomial of degree less than or equal to $k-1$ and $f_j(v) = 0$, $1 \leq j \leq J$, then $v = 0$.*

Then, the quantity

$$\|v\| = |v|_{k,p,\Omega} + \sum_{j=1}^{J} f_j(v)$$

or

$$\|v\| = \left[|v|_{k,p,\Omega}^p + \sum_{j=1}^{J} f_j(v)^p \right]^{1/p}$$

defines a norm on $W^{k,p}(\Omega)$, which is equivalent to the norm $\|v\|_{k,p,\Omega}$.

A proof of this result can be found in [79].

Many useful inequalities can be derived as consequences of the previous theorem. As an example, if Γ_1 is an open, non-empty subset of the boundary $\partial\Omega$, then there is a constant $c > 0$, depending only on Ω such that

$$\|v\|_{1,\Omega} \leq c\left(|v|_{1,\Omega} + \|v\|_{L^1(\Gamma_1)}\right) \quad \forall\, v \in H^1(\Omega).$$

This inequality can be derived by applying Theorem 1.14 with $k = 1$, $p = 2$, $J = 1$ and

$$f_1(v) = \int_{\Gamma_1} |v| \, ds.$$

Therefore,

$$\|v\|_{1,\Omega} \le c\,|v|_{1,\Omega} \quad \forall\, v \in H^1_{\Gamma_1}(\Omega), \tag{1.6}$$

where

$$H^1_{\Gamma_1}(\Omega) = \{v \in H^1(\Omega) : v = 0 \text{ a.e. on } \Gamma_1\}.$$

Hence, the seminorm $|\cdot|_{1,\Omega}$ is a norm on $H^1_{\Gamma_1}(\Omega)$, equivalent to the usual $H^1(\Omega)$-norm $\|\cdot\|_{1,\Omega}$. The inequality (1.6) is a Poincaré-type inequality. In what follows, both $|\cdot|_{1,\Omega}$ and $\|\cdot\|_{1,\Omega}$ will be used as the norm in $H^1_{\Gamma_1}(\Omega)$.

1.4. WEAK FORMULATION OF BOUNDARY VALUE PROBLEMS

Classical solutions of boundary value problems of partial differential equations may not exist even for smooth data (cf. [67, Section 1.1]). The development of the theory of Sobolev spaces and weak formulations eliminates this problem and provides a general framework to derive powerful numerical methods. In this section, we briefly discuss weak formulations of boundary value problems.

We start with the homogeneous Dirichlet boundary value problem of the Poisson equation

$$-\Delta u = f \quad \text{in } \Omega, \tag{1.7}$$

$$u = 0 \quad \text{on } \partial\Omega. \tag{1.8}$$

The standard weak formulation is

$$u \in H^1_0(\Omega), \quad \int_\Omega \nabla u \cdot \nabla v\, dx = \int_\Omega f\, v\, dx \quad \forall\, v \in H^1_0(\Omega). \tag{1.9}$$

Here we assume $f \in L^2(\Omega)$. If $f \in H^{-1}(\Omega)$, then the right hand side of the equation is understood to be the duality pairing $\langle f, v\rangle$ between the spaces $H^{-1}(\Omega)$ and $H^1_0(\Omega)$. The weak formulation (1.9) is derived from (1.7)–(1.8) as follows: First, multiply the equation (1.7) by an arbitrary function v, suitably smooth so that the following calculations are justified, and assumed zero on the boundary. Next, integrate the resulting equation over Ω, and perform an integration by parts on the left hand side to obtain the integral identity

$$\int_\Omega \nabla u \cdot \nabla v\, dx = \int_\Omega f\, v\, dx.$$

Finally, observe that both sides of the integral identity make sense even if we only require $u, v \in H^1(\Omega)$. Together with the zero boundary value condition, we thus require $u, v \in H^1_0(\Omega)$.

Relations between the classical formulation (1.7)–(1.8) and the weak formulation (1.9) are: