Computer Science and Applied Mathematics

FINITE ELEMENT SOLUTION OF BOUNDARY VALUE PROBLEMS

THEORY AND COMPUTATION

O. Axelsson and V. A. Barker

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O. AXELSSON
Department of Mathematics
University of Nijmegen
Nijmegen, The Netherlands

V. A. BARKER
Institute for Numerical Analysis
The Technical University of Denmark
Lyngby, Denmark

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To Anneli and Gunhild

Preface

The purpose of this book is to provide an introduction to both the theoretical and computational aspects of the finite element method for solving boundary value problems for partial differential equations. It is written for advanced undergraduates and graduates in the areas of numerical analysis, mathematics, and computer science, as well as for theoretically inclined workers in engineering and the physical sciences.

Finite element analysis arose essentially as a discipline for solving problems in structural engineering, and its role in that field is still of fundamental importance today. It soon became clear, however, that the method had implications far beyond those originally considered and that it in fact presented a very general and powerful technique for the numerical solution of differential equations. This newer aspect of finite element analysis has been intensively developed in recent years, with the result that at the present time it is problably as important as the traditional engineering applications.

Because a great deal of material on the finite element method has been published, the task of writing a textbook in this area requires basic decisions regarding the choice of topics and depth of treatment. We have chosen to limit the breadth of material severely, concentrating mainly on boundary value problems of the linear, self-adjoint, second-order type. Even within this framework we have made no attempt to be comprehensive. On the other hand, the detailed treatment of the material presented should give the reader sufficient background for reading much of the current literature. Some of this material appears for the first time in book form.

The application of the finite element method to a boundary value problem of the type described above yields a sparse, symmetric system of linear algebraic equations, usually positive definite and often of very high order. Solving such a system is a major computational task in itself, and an important part of the book is devoted to methods for this purpose. One of the most successful, the conjugate gradient method, is analyzed in Chapter 1. This is an example of a minimization method. More specifically, we can associate with a given $N \times N$ positive definite system

$$H\hat{\mathbf{x}} = \mathbf{b}$$

the quadratic functional

$$f(\mathbf{x}) = \tfrac{1}{2}\mathbf{x}^{\mathrm{T}}H\mathbf{x} - \mathbf{b}^{\mathrm{T}}\mathbf{x}, \qquad \mathbf{x} \in R^{N},$$

and show that

$$\min_{\mathbf{x}\in R^N} f(\mathbf{x}) = f(\hat{\mathbf{x}}).$$

Thus, any numerical procedure that minimizes f is per se a method for solving the above system, and this is the case of the conjugate gradient method. In fact, we have chosen to begin the book with the conjugate gradient method because the analysis of quadratic functionals of the above type helps to prepare the reader for the less simple quadratic functionals introduced in Chapters 2 and 3.

The effectiveness of the conjugate gradient method can be much improved by the technique of preconditioning, a topic of current research. Chapter 1 deals with two important kinds of preconditioning, one based on the symmetric successive overrelaxation (SSOR) iterative method for solving a system of equations and the other on a form of incomplete factorization.

Chapter 2 begins the discussion of boundary value problems. It is essentially a review of the classical use of the calculus of variations to establish that the solution of a boundary value problem often minimizes a quadratic functional defined on an infinite-dimensional space of functions. In the case of the simple problem

$$-[p(x)u']' = r(x), \qquad a < x < b, \quad u(a) = u(b) = 0,$$

for example, such a functional is

$$f(u) = \int_a^b [\tfrac{1}{2}p(u')^2 - ru]\,dx, \qquad u \in V,$$

where V is the space of twice continuously differentiable functions vanishing at the endpoints of the interval.

Chapter 3 is an elementary treatment of an advanced topic, namely, the modern trend in boundary value problems with its emphasis on concepts from functional analysis. In the case of the boundary value problem above, for example, we shall see that V can be enlarged to the Sobolev space $\mathring{H}^1(a, b)$, which includes functions with discontinuous first-order derivatives. This relaxation of the continuity requirement turns out to be of fundamental importance for the finite element method.

Chapter 4 presents the Ritz method (and the closely related Galerkin method), which minimizes the quadratic functional associated with a given boundary value problem over some finite-dimensional subspace of the original space of functions. By this process the problem of solving a linear boundary value problem is replaced by the simpler problem of solving a system of linear algebraic equations.

The Ritz (or Galerkin) method becomes the finite element method when the subspace of functions is taken to be the span of a set of finite element basis functions, and this is the subject of Chapter 5. A finite element basis function is a continuous, piecewise polynomial determined from a chosen discretization (called a finite element mesh) of the boundary value problem's domain of definition. In problems with two space variables the elements are usually triangles or rectangles. The success that the finite element method has enjoyed is due in large part to the fact that there is great flexibility in choosing the mesh, particularly when the elements are triangles. This flexibility can be exploited if the domain has an irregular boundary or if the solution is known to change more rapidly in one part of the domain than in another.

A finite element basis function has local support, i.e., it vanishes everywhere outside of a small region in the domain. Because of this property the Ritz–Galerkin system of equations is sparse and can be solved efficiently by the methods described in Chapters 1, 6, and 7.

Chapter 6 is devoted to direct methods (i.e., Gaussian elimination and related methods) for solving a system of linear algebraic equations. A direct method, in contrast to an iterative method, modifies the coefficient matrix in the course of the computation and, when the matrix is sparse, usually introduces fill-in. In the case of finite element problems, both the details of the computer implementation of a direct method and the amount of fill-in produced are very much related to the ordering of nodes in the mesh. Thus, much of the chapter is concerned with various strategies for ordering the nodes and their corresponding computational features.

Chapter 7 continues the analysis of the preconditioned conjugate gradient method begun in Chapter 1, concentrating on applications to finite element problems. After an examination of SSOR preconditioning in this context, a preconditioning based on a modified form of incomplete factorization that is more robust than the unmodified version of Chapter 1 is presented. The second half of the chapter includes techniques for reducing rounding errors in the iterative solution of finite element equations, a discussion of the relative merits of iterative and direct methods for solving such systems, and an account of some recent multigrid methods. Much of the material of this chapter is rather specialized, reflecting some of the directions of current research.

A reading of the book need not follow the order in which topics are presented. In particular, because Gaussian elimination is central for preconditioning by incomplete factorization, the reader, depending on his background, may prefer to read Sections 6.1 and 6.2 before reading the last part of Chapter 1. He could also delay Chapter 1 until after Chapter 5 or 6.

How the reader chooses to divide his time between the theoretical and computational parts of the book will be very much a matter of taste. Some, for example, may wish to skip over most of the mathematical details of Chapters 2 and 3 and the last half of Chapter 5. In fact, much of the computational material could make independent reading.

Regarding computer implementation of the various methods presented, listings of program code have been by and large avoided. On the other hand, we have not hesitated to describe algorithms in an informal computer-oriented language when convenient. In some cases, details of implementation have been left to the exercises. Considerable effort has been put into providing a broad set of exercises covering most of the topics presented.

The reader's background should include familiarity with linear algebra and basic analysis. In particular, he should be acquainted with matrix and vector norms and with the elementary properties of the eigenvalue problem for symmetric matrices. Naturally, the more he knows about boundary value problems for differential equations, the better.

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List of Symbols

Vectors and Matrices

R	field of real numbers
R^N	real N-dimensional vector space
$\mathbf{x} = [x_1, x_2, \ldots, x_N]^T$	typical element of R^N
$\mathbf{x}^T\mathbf{y} = \sum_{i=1}^N x_i y_i$	Euclidean inner product of $\mathbf{x}$ and $\mathbf{y}$
$\lVert\mathbf{x}\rVert = (\mathbf{x}^T\mathbf{x})^{1/2}$	Euclidean norm of $\mathbf{x}$
$\lVert\mathbf{x}\rVert_\infty = \max_i \lvert x_i\rvert$	maximum norm of $\mathbf{x}$
$H = [h_{ij}]$	typical $N \times N$ real matrix
$\lambda_1, \lambda_2, \ldots, \lambda_N$	eigenvalues of H, where $0 \le \lvert\lambda_1\rvert \le \lvert\lambda_2\rvert \le \cdots \le \lvert\lambda_N\rvert$
$\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$	eigenvectors of H ($H\mathbf{v}_i = \lambda_i\mathbf{v}_i$)
$\rho(H) = \lvert\lambda_N\rvert$	spectral radius of H
$\lVert H\rVert = \rho(H^TH)^{1/2}$	spectral norm of H ($H^T = H \Rightarrow \lVert H\rVert = \lvert\lambda_N\rvert$)
$\lVert H\rVert_\infty = \max_i \sum_{j=1}^N \lvert h_{ij}\rvert$	maximum norm of H
$\kappa(H) = \lVert H\rVert \cdot \lVert H^{-1}\rVert$	spectral condition number of H ($H^T = H \Rightarrow \kappa(H) = \lvert\lambda_N\rvert/\lvert\lambda_1\rvert$)
$(\mathbf{x}, \mathbf{y})_H = \mathbf{x}^T H\mathbf{y}$	energy inner product of $\mathbf{x}$ and $\mathbf{y}$, where H is symmetric positive definite
$\lVert\mathbf{x}\rVert_H = (\mathbf{x}, \mathbf{x})_H^{1/2}$	energy norm of $\mathbf{x}$
$H = LU$	unsymmetric Gaussian factorization of H
$H = LDL^T$	symmetric Gaussian factorization of H, where H is symmetric
$H = \tilde{L}\tilde{L}^T$	Cholesky factorization of H, where H is symmetric positive definite
$H = LU + R$, $H = LDL^T + R$, $H = \tilde{L}\tilde{L}^T + R$	incomplete factorizations of H
$m(i)$	column number of the first nonzero entry in the ith row of H

$n(i)$	column number of the last nonzero entry in the ith row of H
$w(H) = \max_{2 \le i \le N} [i - m(i)]$	half-bandwidth of a symmetric matrix H
$e(H) = \sum_{i=2}^{N} [i - m(i)]$	envelope parameter of a symmetric matrix H
$f(\mathbf{x})$	typical functional defined on $X \subseteq R^N$
$\mathbf{g}(\mathbf{x})$	gradient vector of f with components $g_i = \partial f/\partial x_i$, $i = 1, 2, \ldots, N$
$H(\mathbf{x})$	Hessian matrix of f with entries $h_{ij} = \partial^2 f/\partial x_i \partial x_j$, $i, j = 1, 2, \ldots, N$

Functions

(a, b)	$\{x \in R; a < x < b\}$
$[a, b]$	$\{x \in R; a \le x \le b\}$
n	number of space dimensions
Ω	open set in R^n
Γ	boundary of Ω
$\bar{\Omega}$	$\Omega \cup \Gamma$
u	typical real function defined on $\bar{\Omega}$
u_ν	outer normal derivative of u on Γ
u_τ	tangential derivative of u on Γ in the counter-clockwise sense
$u^{(\alpha)}$	multi-index notation for the partial derivative $\partial^{\lvert\alpha\rvert} u/\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \partial x_n^{\alpha_n}$, where $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ and $\lvert\alpha\rvert = \sum_{i=1}^{n} \alpha_i$
Δu	$\sum_{i=1}^{n} \partial^2 u/\partial x_i^2$
$L_2(\Omega)$	space of real square-integrable functions on Ω
$(u, v) = \int_\Omega uv \, d\Omega$	$L_2(\Omega)$ inner product of u and v
$\lVert u \rVert = (u, u)^{1/2}$	$L_2(\Omega)$ norm of u
$H^k(\Omega)$	Sobolev space of real functions defined on Ω with square-integrable generalized derivatives of order $\le k$
$(u, v)_k = \sum_{\lvert\alpha\rvert \le k} \int_\Omega u^{(\alpha)} v^{(\alpha)} \, d\Omega$	Sobolev [or $H^k(\Omega)$] inner product of u and v
$\lVert u \rVert_k = (u, u)_k^{1/2}$	Sobolev [or $H^k(\Omega)$] norm of u

$[u, v]_k = \sum_{\lvert\alpha\rvert=k} \int_\Omega u^{(\alpha)} v^{(\alpha)}\, d\Omega$	Sobolev semi-inner product of u and v
$\lvert u \rvert_k = [u, u]_k^{1/2}$	Sobolev seminorm of u
$C^k(\Omega)$, $C^k(\bar{\Omega})$	space of real, k times continuously differentiable functions on Ω and $\bar{\Omega}$, respectively; $C(\Omega) = C^0(\Omega)$, $C(\bar{\Omega}) = C^0(\bar{\Omega})$
$\lVert u \rVert_\infty = \max_{\mathbf{x}\in\bar{\Omega}} \lvert u(\mathbf{x}) \rvert$	maximum norm of u, where $u \in C(\bar{\Omega})$
$\mathring{H}^k(\Omega)$	completion with respect to the norm $\lVert \cdot \rVert_k$ of the subset of $C^k(\Omega)$ with compact support on Ω
$a(u, v)$	typical bilinear form
$(u, v)_{\mathscr{L}} = a(u, v)$	energy inner product of u and v, where $a(\cdot, \cdot)$ is symmetric and coercive
$\lVert u \rVert_{\mathscr{L}} = (u, u)_{\mathscr{L}}^{1/2}$	energy norm of u
$P_k(\bar{\Omega})$	space of polynomials of degree $\leq k$ defined on $\bar{\Omega}$
$T_k(x)$	Chebyshev polynomial of degree k

Finite Elements

L	number of elements in a finite element mesh
M	number of nodes in a finite element mesh
T	number of nodes in a single element
e_l, $l = 1, 2, \ldots, L$	elements
$N_i = (x_i, y_i)$, $i = 1, 2, \ldots, M$	nodes
$i_r^{(l)}$, $r = 1, 2, \ldots, T$	node numbers of nodes in e_l
$\phi_i(x, y)$, $i = 1, 2, \ldots, M$	global basis functions (defined on $\bar{\Omega}$)
$V_M = \mathrm{SPAN}\{\phi_1, \phi_2, \ldots, \phi_M\}$	finite element space
$u_I = \sum_{i=1}^{M} u(N_i)\phi_i$	V_M interpolant of u
$\phi_r^{(l)}(x, y)$, $r = 1, 2, \ldots, T$	local basis functions (defined on e_l)
$\tilde{e}$	standard element
$\tilde{\phi}_r(\tilde{x}, \tilde{y})$, $r = 1, 2, \ldots, T$	standard local basis functions (defined on $\tilde{e}$)
$(\tilde{x}^{(m)}, \tilde{y}^{(m)})$, $m = 1, 2, \ldots, Q$	integration points
w_m, $m = 1, 2, \ldots, Q$	integration weights
$K^{(l)}$, $l = 1, 2, \ldots, L$	element stiffness matrices

$M^{(l)}$, $l = 1, 2, \ldots, L$	element mass matrices
$\mathbf{G}^{(l)}$, $l = 1, 2, \ldots, L$	element vectors
K	global stiffness matrix
M	global mass matrix
$\mathbf{G}$	global vector
$\mathbf{G}^*$	global vector modified by a Dirichlet boundary condition
h	greatest element edge length in the mesh

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