Analysis of Global Expansion Methods: Weakly Asymptotically Diagonal Systems

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London New York Toronto Sydney San Francisco

ACADEMIC PRESS INC. (LONDON) LTD 24-28 Oval Road London NW1

US edition published by ACADEMIC PRESS INC. 111 Fifth Avenue New York, New York 10003

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British Library Cataloguing in Publication Data.

Delves, L. M.

Analysis of global expansion methods. – (Computational mathematics and applications).

- 1. Differential equations Asymptotic theory
- 2. Integral equations
- 3. Matrices
- I. Title II. Freeman, T. L. III. Series

515.3'5 QA371

ISBN 0-12-208880-8 LCCCN 80-42084

Preface

The study of Weakly Asymptotically Diagonal systems originated in an attempt to analyse the convergence of expansion methods for differential and integral equations of "global" type; that is, methods which employ expansions of the form

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$$f(x) = \sum_{i=1}^{N} a_i^{(N)} h_i(x),$$

where the $h_i(x)$ have global rather than local support and are typically chosen to be orthogonal polynomials in an appropriate set of variables. For a linear problem, such methods lead to a set of linear equations for the coefficients $a_i^{(N)}$, $i=1,\ldots,N$, and it is possible to treat both the convergence and the stability properties of the method by analysing the structure of the matrix and right-hand side of these equations. Such an approach has the advantage that these properties are then characterised directly in terms of quantities which are available without additional cost during the course of the calculations: the error estimates which result are cheap to compute.

For the analysis to be of general use, it is necessary to abstract the essential structure of the equations, and to analyse the class of matrices having this structure. The definition of a Weakly Asymptotically Diagonal (WAD) matrix arises directly from this necessity. Historically, two subclasses of WAD matrices were introduced first: matrices of type A, which closely model the equations that arise from Fredholm integral equations, and type B, which model differential equations.

These subclasses yield a rather straightforward analysis of the convergence and stability properties of global expansion methods for one-dimensional problems, together with cheaply computable and very effective error estimates for such methods. Systems of type A in particular yield a rather simple theory, which is discussed in detail in Chapter 2.

The more abstract general WAD definitions arise from a natural wish to broaden the class of problems covered by the analysis as much as possible, and to formalise the essential results contained in the rather specific theorems of type A and type B systems. It appears that this can be achieved in quite a natural manner, and a considerable body of analysis has grown up for WAD matrices. Although it is by no means complete, it seems worthwhile to bring together the available results together with some of their applications to expansion methods; the result is this book, which splits naturally into three sections.

The theory and numerical analysis of WAD systems is discussed in Chapters 1-8; we hope that the ordering chosen, and the examples given, illustrate sufficiently the analysis to motivate this detailed study. The third section, Chapters 12-14, discusses applications of the theory to the solution of integral and differential equations. Space considerations limit the detail that can be given in these chapters. However, it is our hope that they, and also Chapter 8 on the numerical analysis of WAD systems, form a practical justification for Chapters 1-7: namely, that the study of WAD systems, and the insight which these systems give into the structure of global expansion methods, has led directly to the development of improved algorithms and to cheap and effective error estimates for a wide class of problems. The error estimates depend on the parameters of the WAD systems, and these parameters can themselves be directly estimated during the calculations. They can, however, also be related to the analytic properies (the smoothness) of the coefficients in the equation being solved. Section 2, Chapters 9-11, is devoted to the analysis of the convergence properties of orthogonal expansions, and discusses this relationship in detail. These chapters thus form a bridge between the abstract WAD theory and its applications in Chapters 12-14. They also form a bridge between the basis—dependent analysis of this book, and the more common basis—independent analysis of the convergence of variational and Galerkin methods in which the assumed smoothness properties of the equations appear directly.

This book contains a number of new and extended results, but its main purpose is to draw together previously published results. We are grateful to all of our colleagues who have worked in this field, and particularly to Drs M. Bain, K. O. Mead and F. A. Musa, for permission to draw upon their theses and published work, as listed in the references, as well as for many discussions. Without their collaboration and cooperation, this book could not have been written. Responsibility for any errors which remain in it, however, rests with us. We would also like to acknowledge with gratitude the patience and forbearance of Miss K. Anderson and Mrs G. M. Eyres, in seeing us through successive drafts.

Liverpool & Manchester March 1981

L. M. Delves T. L. Freeman

Contents

Preface

Intr	Eigenvalue convergence notivation and Motivation		
1.1	Introduction on pergent on the state of the state o	6.3.	3
1.2	Galerkin methods for linear operator equations	4.0	4
1.3	Convergence and error analysis of Galerkin methods	65.	10
1.4	The special role of orthogonal expansions		12
1.5		6.6.	15
	Numerical example		
Asv	mptotically Diagonal Systems of Type A		
2.1			19
2.2			k .
			20
2.3	Behaviour of a ^(N) and b		23
	Convergence of variational or Galerkin calculations		26
		· Land	35
2.6	Numerical examples A V. 1997.	nukl	36
Wea	akly Asymptotically Diagonal Systems	CR	
3.1	Introduction and in the interior and in the interior and the interior		41
3.2	A class of non-singular matrices	·1 8	42
3.3	Bounds on the inverses of certain matrices	.2 8	46
3.4	Infinite matrices	- A - R	49
	Behaviour of $\mathbf{a}^{(N)}$ and \mathbf{b} .		
	1.1 1.2 1.3 1.4 1.5 Asy 2.1 2.2 2.3 2.4 2.5 2.6 Wes 3.1 3.2 3.3 3.4	Introduction and Motivation 1.1 Introduction 1.2 Galerkin methods for linear operator equations 1.3 Convergence and error analysis of Galerkin methods 1.4 The special role of orthogonal expansions 1.5 An example Asymptotically Diagonal Systems of Type A 2.1 Introduction 2.2 Triangular decomposition of symmetric AD matrices of type A 2.3 Behaviour of a ^(N) and b 2.4 Convergence of variational or Galerkin calculations 2.5 A theorem based on a variational principle 2.6 Numerical examples Weakly Asymptotically Diagonal Systems 3.1 Introduction 3.2 A class of non-singular matrices 3.3 Bounds on the inverses of certain matrices 3.4 Infinite matrices 3.5 Behaviour of a ^(N) and b	Introduction and Motivation 1.1 Introduction 1.2 Galerkin methods for linear operator equations 1.3 Convergence and error analysis of Galerkin methods 1.4 The special role of orthogonal expansions 1.5 An example Asymptotically Diagonal Systems of Type A 2.1 Introduction 2.2 Triangular decomposition of symmetric AD matrices of type A 2.3 Behaviour of a ^(N) and b 2.4 Convergence of variational or Galerkin calculations 2.5 A theorem based on a variational principle 2.6 Numerical examples Weakly Asymptotically Diagonal Systems 3.1 Introduction 3.2 A class of non-singular matrices 3.3 Bounds on the inverses of certain matrices 3.4 Infinite matrices 3.5 Behaviour of a ^(N) and b

Perficular Classes of Weeldy Asymptotically Diagonal

Scapility Analysis tol Wealthy Jayonprevietlly Diagonal

Section 1: Theory of WAD Systems 1 and wheeping

Consymmetric services

vii

viii Contents

4.	222	ticular Classes of Weakly Asymptotically Diagonal tems	
	4.1	Introduction	63
	4.2	Type B systems	64
	4.3	Type C systems	67
	4.4	Type E systems	68
	4.5	Unsymmetric systems	75
5.		bility Analysis of Weakly Asymptotically Diagonal	
		tems	
	5.1		80
, 3	5.2	Bounds on L	81
	5.3		82
	5.4	Bounds on the individual elements of δa	86
	5.5	The stability of f_N	91
6.	Eige	envalue Problems CAW to yroad? : nottes2	
	6.1	Introduction	101
	6.2	Eigenvalue convergence	102
8	6.3	Eigenvector convergence no laubouted .	110
34	6.4	Prediction coefficients for the eigenvectors .	111
0.1	6.5	An alternative bound on the convergence rate of the dom-	
		inant eigenvalue and pas la roport to to alor la bega off :	115
15	6.6	Stability against round-off errors	118
	6.7		120
7.		ck Weakly Asymptotically Diagonal Systems	
.81	1.1		123
		Block triangular decomposition of BWAD matrices .	126
	7.3	Bounds on the inverse of a BWAD matrix. A	130
	7.4	Behaviour of a ^(N) and b . d bus (Na lo juoiyudos)	134
35	7.5	Convergence of Galerkin calculations	136
8.		merical Methods for Weakly Asymptotically Diagonal	2.5
		trices	
	8.1	Introduction	144
2.70	8.2		144
41		Iterative solution of sets of equations	147
	8.4	Practical applications 240,116.1 15 byship-non to best A .	150
40	8.5	Asymptotic estimates of the solution vector	152
	8.6	The least squares solution of over-determined systems .	158
-88		Eigenvalue problems	159
	88	Calculation of eltenoisaluolas distribution of eltenoisaluolas	164

		Section 2: Orthogonal Expansions		a initi		14,
255		MO	iloubo	etril b	41	
		Convergence of Orthogonal Expansions				
	Inte		eir nia	all E	14.	
250		methods noitoubortnI	ticular	4 Pas	bi	169
		Classical Fourier expansions				1/2
198	9.3	Sturm-Liouville eigenfunction expansion se		a finit	e	7. 9.
		interval $[a, b]$				174
073		Expansions in Jacobi polynomials .		ydqes	goi	177
		Convergence in the uniform norm .			٠	185
	9.6	Transformation of variables	٠,		• 30	185
10.	Orth	nogonal Expansions on Infinite Intervals				
		Eigenfunction expansions on the semi-infini		rval		188
		Expansions on [0, ∞): Laguerre polynomial				189
	10.3	Expansions on $(-\infty, \infty)$. Hermite polynomial	ials			195
		Examples				198
	10.5	Alternative expansion sets		٠,	٠	200
11.	The	Convergence of Multi-dimensional Expar	sions			
		Introduction				206
	-11.2	Eigenfunction expansions				207
		Generalised Green's theorem				210
	11.4	A brute force method	*			214
		Section 3: Applications				
12.	The	Galerkin Solution of Integral Equations				
		Introduction				219
		Expansions in Legendre polynomials .				221
		Expansions in Chebyshev polynomials				227
		Singular integral equations				230
13.	Glol	oal Expansion Methods for Ordinary	Diffe	erentia	al	
		ations				
		Introduction				236
		A simple example: the half-range sine expa	nsion			237
						240
		Expansions in ultraspherical harmonics				242
		The choice of weight function: polynomial	expans	sions		246
		Inhomogeneous boundary conditions .				250
		Least squares or Galerkin?				253

×					Contents
14 Partial	Differential Equa	tions	n 2: Ortho	Sectio	

14.	Part	ial Diffe	erentia	I Equ	ation	sagar	2: Ord	Section			
	14 4	Introdu	iction								255
	14.2	The m	odel p	robler	n	enego	nimu ii	gence c	course	eur	255
	14.3	Block	matrix	form					lev	iețal	257
169	14.4	Particu	lar me	thods					Introdu	9.1	260
								shoot is		7.6	
App	pendi	x: Som	e seri	es bo	unds	uncio	inages :	Ljonestle Lja, bj	Studen-	€.0	261
Bib	liogra	vhq			zkim	ranglor	infoseli.	ni anon	Едраня	1.0	270
185		,								9,5	
Ind	ex										
			8								
881											
195								no enoi			
					2 140						
							most i			erlT	
						X 97					
						2777					
214											
							etion 3				
				startine.						1.6-17	
							110-110				
122											
				EIBL							
				BIN(D)							
									snois		
237								le exam			
240											
242											
		SHOISHI									
250				8.0	onipu						

Section 1 Theory of WAD Systems

Section 1

Theory of WAD Systems

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1.2 Caleridin methods for linear operator equations

1.2.1 The Calerbin formalism

form f, which approximates it Thus

Let R be a Hilbert space with inner product (\cdot, \cdot) and $\mathcal{Z} : R \to R$ a linear operator defined on R (or perhaps a subspace of R). Let g be a known element of R, and f the solution (assumed to exist and to be unique in G) of the linear operator equation

Introduction and Motivation

1.1 Introduction

This book is primarily concerned with the analysis of a class of infinite matrices: the class of Weakly Asymptotically Diagonal (WAD) matrices of the title. This analysis is interesting in its own right; however, the major interest lies (for the authors at least) in the application of the theory to problems in the general field of approximation theory. WAD matrices arise naturally when global or global element expansion methods are used to solve numerically a wide class of problems which involve integral and differential equations in one or more dimensions; the WAD assumptions were in fact introduced in order to model the structure of the matrices that arise from these problems. In this chapter we therefore try to motivate the analysis of Chapters 2-7 by giving a brief discussion of such methods. We demonstrate by example their main source of interest: the possibility of obtaining very rapid convergence; convergence which in "suitable" cases is much more rapid than that attainable with a conventional finite difference or finite element approach. However, rapid convergence is of little use in practice unless it can be recognised: what is needed is a computable error estimate which reflects the actual error as faithfully as possible while adding as little as possible to the cost of the calculations. The provision of such error estimates is one of the main achievements of the WAD theory developed here. The estimates depend on an analysis of the structure of the defining equations for the expansion method; this structure is displayed in a simple case in the example of Section 1.5. Once the structure is understood, surprisingly simple and effective error estimates follow. In addition, the structure suggests efficient ways of both setting up and of solving the defining equations; see Chapters 8 and 12–14 for a discussion of the savings which can be made.

1.2 Galerkin methods for linear operator equations

1.2.1 The Galerkin formalism

Let R be a Hilbert space with inner product (\cdot, \cdot) and $\mathcal{L}: R \to R$ a linear operator defined on R (or perhaps a subspace of R). Let g be a known element of R, and f the solution (assumed to exist and to be unique in R) of the linear operator equation

$$\mathscr{L}f = g. \tag{1.2.1}$$

An expansion method introduces a complete set $\{h_i\}$, i = 1, 2, ..., of elements in R, and expansions for the exact solution of (1.2.1) and the truncated form f_N which approximates it. Thus

$$f = \sum_{i=1}^{\infty} b_i h_i \tag{1.2.2}$$

$$f_N = \sum_{i=1}^{N} a_i^{(N)} h_i. {(1.2.3)}$$

The method also provides an algorithm for computing the coefficients $a_i^{(N)}$ in the approximate solution. Many algorithms can be constructed; we consider here only the unsymmetric Galerkin method or method of moments, which introduces a second set of elements $\{\hat{h}_i\}$ and computes $\mathbf{a}^{(N)} = (a_i^{(N)})$ as the solution of the $N \times N$ linear system

$$\mathbf{La}^{(N)} = \mathbf{g} \tag{1.2.4}$$

where the matrix L and vector g are defined by

$$L_{ij} = (\hat{h}_p \mathcal{L}h_j), \quad i, j = 1, ..., N,$$
 (1.2.5)

$$g_i = (\hat{h}_i, g), \qquad i = 1, ..., N.$$
 (1.2.6)

In practice, the sets $\{\hat{h}_i\}$, $\{h_i\}$ may be related; for example, we may choose $\hat{h}_i = \mathcal{L}h_i$ (method of least squares) or $\hat{h}_i = wh_i$ (weighted Galerkin). The choice $\hat{h}_i = h_i$ yields the symmetric Galerkin technique; we shall use the generic term Galerkin method, the precise choice of \hat{h}_i being evident from the context.

The use of a Galerkin technique for numerical calculations raises a number of interesting and interrelated questions:

(i) Posing the problem

How do we pose a given type of problem in the form (1.2.1)? In particular, for differential equations, this question usually reduces to: How do we treat the boundary conditions?

(ii) Choosing the expansion set

How do we choose the basis set $\{h_i\}$ in (1.2.2), (1.2.3), and the companion set $\{\hat{h}_i\}$ in (1.2.5), (1.2.6)? How does this choice affect the accuracy of the calculation? The cost of the calculation? The stability against numerical or round-off errors? The convenience?

(iii) Computing the solution

Setting up the matrix problem (1.2.4) usually involves providing numerical approximations to the inner products involved; the choice of approximation can crucially affect both the accuracy obtained and the time taken. For the large systems which result from multi-dimensional problems, the methods used to solve (1.2.4) are also important since the solution time can be as great as or greater than the time taken to form the equations.

(iv) Analysing the errors

Three classes of numerical error can be distinguished in a Galerkin calculation:

- (a) Truncation errors These stem from the truncation of (1.2.2) after N terms.
- (b) Discretisation errors

 These stem from the differences $b_i a_i^{(N)}$, $i_i = 1, 2, ..., N$.
- (c) Quadrature errors

Given that we approximate the inner products involved (using quadrature rules) we in fact solve not (1.2.4) but the perturbed system

$$(\mathbf{L} + \delta \mathbf{L})(\mathbf{a}^{(N)} + \delta \mathbf{a}^{(N)}) = \mathbf{g} + \delta \mathbf{g}, \qquad (1.2.7)$$

these perturbations yielding an additional source of error, $\delta a^{(N)}$.

1.2.2 An example

We provide a partial answer to questions (i) and (ii) above by means of an example. Consider the real, linear Fredholm integral equation of the second kind

$$f(x) = g(x) + \lambda \int_a^b K(x, y) f(y) dy.$$
 (1.2.8)

Under suitable assumptions (on the kernel λK , and driving term g), this equation has a unique solution. If we choose an inner product on the

[†] For example: if g(x) is continuous in [a, b], K(x, y) is continuous in $[a, b] \times [a, b]$, and λ is not a characteristic value of (1.2.8), then there exists a unique continuous solution f(x).

(ii) Choosing the expansion set

interval [a, b]:

How do we choose the basis set
$$M_1$$
 f_1 f_2 f_3 f_4 f_5 f_5 f_6 f_6

and set

$$\hat{h}_i(x) = h_i(x), \quad i = 1, 2, \dots,$$
 (1.2.10)

then (1.2.5), (1.2.6) takes the form [20, 12.1] moldary about our antibody

$$L_{ij} = \int_{a}^{b} w(x)h_{i}(x)h_{j}(x) dx - \lambda \int_{a}^{b} w(x)h_{i}(x) \int_{a}^{b} K(x, y)h_{j}(y) dy dx \qquad (1.2.11)$$

$$g_i = \int_a^b w(x)h_i(x)g(x) dx$$
. The solution of the solution

Equations (1.2.4), (1.2.11), (1.2.12) are the formal defining equations for the Galerkin method applied to the problem (1.2.8). The same equations result if we choose the *unweighted inner product*

$$(f_1, f_2) = \int_a^b f_1(x) f_2(x) \, dx \qquad (1.2.12a)$$

and set

$$\hat{h}_i(x) = w(x)h_i(x), \quad i = 1, 2, \dots$$
 (1.2.12b)

A numerical method results from these defining equations once we:

- (a) specify the basis set $\{h_i\}$;
- (b) specify how the integrals are to be performed.

We are not concerned here with (b) (but see Chapter 12). The choice (a) lies primarily between *local* and *global* bases; we can informally describe these as follows:

Local basis and shound (iii) bear (i) aroutesup of reward learning a shround sW

We split the region $a \le x \le b$ into intervals of width h. On each subinterval [a+mh, a+(m+1)h] the approximate solution $f_N(x)$ is taken to be a polynomial of fixed degree p. Continuity conditions may be imposed across subinterval boundaries (for example, a *spline basis* results if $f_N(x)$ is constrained to have p-1 continuous derivatives on [a, b]). Convergence is obtained by letting $h \to 0$ for fixed p.

This description of $f_N(x)$ is not in terms of an expansion of the form (1.2.3), but for any choice of p and of continuity constraints, it can be put in that form. For example, if p = 1 (piecewise linear approximation) and $f_N(x)$ is constrained to be continuous on [a, b], the description can be rephrased as follows:

Define the hat function $Hat_i(x)$:

Hat_i(x) = 0,
$$x \le a + (i - 1)h$$

$$= \frac{x - a - (i - 1)h}{h}, \quad a + (i - 1)h < x \le a + ih$$

$$= \frac{a + (i + 1)h - x}{h}, \quad a + ih < x \le a + (i + 1)h$$

$$= 0, \qquad x > a + (i + 1)h$$

$$h = (b - a)/N. \qquad (1.2.13)$$
Thus, Hat_i(x) is zero except on the interval $[a + (i - 1)h, a + (i + 1)h]$ and

Thus, $\operatorname{Hat}_{i}(x)$ is zero except on the interval [a + (i-1)h, a + (i+1)h] and is linear over the two halves of this interval, with discontinuous first derivative at x = a + ih, and at a + (i-1)h, a + (i+1)h. Now choose as basis

$$h_i(x) = \text{Hat}_i(x), \quad i = 1, ..., N.$$
 (1.2.14)

Global basis Insurance and it is salue for the exponent size of the exponent

The local basis described above has the feature that each of the basis functions $\operatorname{Hat}_i(x)$ depends explicitly on N, and has local support; that is, is zero everywhere except over a small subinterval of [a,b]. A global basis is one in which the basis functions have support over the whole region; in practice, they are also chosen to be independent of N. Within these restrictions, many choices are available. The most common choice is to take $f_N(x)$ to be a polynomial of degree N-1 in x.

We can clearly achieve this in a number of ways; for example, the choice

well be more expensive everall. Further, techniques exist for improvin bns

$$h_{i}(x) = T_{i-1} \left(\frac{2x - (a+b)}{b-a} \right), \quad i = 1, 2, ..., \tag{1.2.16}$$

where $T_k(z)$, $-1 \le z \le 1$, is a Chebyshev polynomial of degree k, and each defines a polynomial approximating function $f_N(x)$; we show in Section 1.3 that these choices are in fact equivalent in the sense that, if quadrature and round-off errors are ignored, they will yield the same solution $f_N(x)$.

The choice between *local* and *global* basis is crucial; the two types lead to quite different numerical techniques both for setting up and for solving the Galerkin equations, and to quite different types of error analysis. They also perform quite differently in practice, as the following example demonstrates.

In (1.2.8), we take

$$\lambda K(x, y) = e^{xy}$$

$$g(x) = e^{x} - (e^{x+1} - 1)/(x+1)$$

$$a = 0, b = 1.$$
(1.2.17)

Then the exact solution of (1.2.8) is

$$f(x) = e^x. (1.2.18)$$

Table 1.1 shows the maximum errors, $||f - f_N||_{\infty}$, obtained using expansion methods with the expansion sets (1.2.14) and (1.2.16).

Looking first at the results using a local expansion, we remark that the errors reduce only relatively slowly as N increases. The results given are in fact well fitted by the form

$$||f - f_N|| \sim CN^{-p}, \quad p = 2,$$

and it is a simple matter to predict this value for the exponent p in advance: it is related to the continuity of the expansion set $\{Hat_i(x)\}$ used, and not at all to the problem being solved, provided that this is "smooth enough". It is more difficult to predict the amplitude C; still, it is certainly an advantage of local methods that the behaviour of the error can be predicted, and hence checked.

Looking next at the global expansion results, we see that very rapid convergence is obtained; for this problem, there is no doubt that the global method is preferable. This rapid convergence is typical of that achieved with a global polynomial basis for problems which have "smooth" solutions. Of course, not all problems are of this type. When the solution is "nonsmooth", a global basis may converge no faster than a local basis, and may well be more expensive overall. Further, techniques exist for improving the performance of both types of expansion. For example, extrapolation procedures such as the "deferred approach to the limit" may be applied to increase the convergence rate of a local calculation, while we may choose to subdivide the region [a, b] into two or more subintervals and apply a global expansion over each subinterval, to improve the performance of a global method. It is not the purpose of this book to argue for or against the use of global as opposed to local bases. Instead, we note the interestingly fast convergence which can be achieved, and ask the question: can this error be predicted in practice for a global method, as it can for a local method? In particular, we would like to provide error estimates for a global expansion method which are cheaply computable and realistic. It transpires that such an analysis of some generality can be given, provided that we limit attention to orthogonal bases as typified by (1.2.16); fortunately, the use of such bases,