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SPARSE MATRICES

numerical aspects with applications for scientists and engineers

U. Schendel

SPARSE MATRICES:
Numerical Aspects with Applications for Scientists and Engineers

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ELLIS HORWOOD LIMITED
Publishers · Chichester

Halsted Press: a division of
JOHN WILEY & SONS
New York · Chichester · Brisbane · Toronto

This English edition first published in 1989 by
ELLIS HORWOOD LIMITED
Market Cross House, Cooper Street,
Chichester, West Sussex, PO19 1EB, England
The publisher's colophon is reproduced from James Gillison's drawing of the ancient Market Cross, Chichester.

Distributors:
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JACARANDA WILEY LIMITED
GPO Box 859, Brisbane, Queensland 4001, Australia
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JOHN WILEY & SONS CANADA LIMITED
22 Worcester Road, Rexdale, Ontario, Canada
Europe and Africa:
JOHN WILEY & SONS LIMITED
Baffins Lane, Chichester, West Sussex, England
North and South America and the rest of the world:
Halsted Press: a division of
JOHN WILEY & SONS
605 Third Avenue, New York, NY 10158, USA

This English edition is translated from the original German edition *Sparse matrizen,* published in 1977 by R. Oldenbourg, Munich, © the copyright holders.

British Library Cataloguing in Publication Data
Schendel, U. (Udo)
Sparse matrices: numerical aspects with applications for scientists and engineers.
1. Algebra. Sparse matrices. Applications
I. Title II. Series
512.9'434

Library of Congress CIP data available

ISBN 0–7458–0635–X (Ellis Horwood Limited)
ISBN 0–470–21406–6 (Halsted Press)

Printed in Great Britain by Hartnolls, Bodmin

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Numerical Aspects with Applications for Scientists and Engineers

MATHEMATICS AND ITS APPLICATIONS

Series Editor: G. M. BELL, Professor of Mathematics, King's College London (KQC), University of London

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Mathematics and its applications are now awe-inspiring in their scope, variety and depth. Not only is there rapid growth in pure mathematics and its applications to the traditional fields of the physical sciences, engineering and statistics, but new fields of application are emerging in biology, ecology and social organization. The user of mathematics must assimilate subtle new techniques and also learn to handle the great power of the computer efficiently and economically.

The need for clear, concise and authoritative texts is thus greater than ever and our series will endeavour to supply this need. It aims to be comprehensive and yet flexible. Works surveying recent research will introduce new areas and up-to-date mathematical methods. Undergraduate texts on established topics will stimulate student interest by including applications relevant at the present day. The series will also include selected volumes of lecture notes which will enable certain important topics to be presented earlier than would otherwise be possible.

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Preface

This book has developed from lectures held at the Free University and Technical University of Berlin. Numerous talks with engineers have shown that there is a need to impart knowledge on large, sparse matrices and the mathematical methods which use these matrices. In this connection it is of great importance that it is only the combined effect of mathematical methods and digital computers which produces the effect of the chosen algorithm. The present book has been written with the intention to fill a gap by dicussing this relationship by means of some methods and by supporting it with examples.

In the selection of material the emphasis was put on numerical methods which belong to the classical, current procedures of numerical mathematics and which have already proved their efficiency in practical use; we did not aim at completeness of all possible procedures. The aim was rather to stress the typical features of the described methods and to achieve a better comprehension of the questions arising in connection with sparse matrices.

A mathematical representation has been chosen which will enable natural scientists, engineers and students of the natural sciences to find access to these problems. Knowledge in the programming in a higher computer language and basic knowledge in numerical mathematics are prerequisite. In particular, this book has been written for readers who work outside universities in practical fields and who want to get a general idea of the topic of sparse matrices.

Large parts of this book have already been published by R. Oldenbourg Publishers, Munich-Vienna.

The idea to translate the German version into English has led to a revision and an extension of the contents. The field of sparse matrix problems has received many a fresh impetus in the last few years.

My colleague, Mr. J. Brandenburger, has contributed essentially in revising and translating the German version of this book. He also produced the camera-ready copy by the word processing system LaTeX. The translation itself is mainly due to Mr. W. Pourie. I want to express to them my particular gratitude for their good cooperation.

Besides, I want to express my thanks to my colleague, Mr. B. Conolly, Queen Mary College, London, for the pains he took in critically reading and polishing the English translation.

Finally I want to thank the Ellis Horwood Publishing Company, London, for their good and sympathetic cooperation.

Berlin, August 1988 U. Schendel

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1 Introduction

For about 20 years the different aspects of sparse matrices have been receiving increasing attention. Several important international conferences have taken place on sparse matrices and their applications with a wide range of topics.

In addition, there have been a number of smaller conferences about specific problems of sparse matrices like QR-methods, structural analysis, power distribution systems, circuit design and others. In numerical analysis most areas, but in particular eigenvalue problems, integral equations, linear and nonlinear equations, linear programming, ordinary and partial differential equations have been covered. In mathematics in a wide sense combinatorics, computing, graph theory and statistics are dealt with, too.

All these special problems lead to a matrix $A := [a_{ik}]$, $A \in \mathbb{R}^{m \times n}, \mathbb{C}^{m \times n}$, whose number r of elements a_{ik} with $a_{ik} \neq 0$ is small in relation to the total number $n \times m$ of all matrix elements.

Effectiveness of work with these matrices requires:

- special numerical algorithms that take account of the sparseness
- special storage techniques
- special programming techniques.

These requirements arise from the necessity for

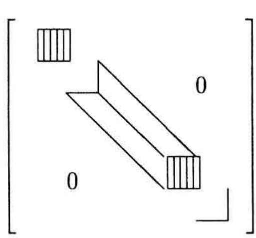
- the results to be numerically acceptable
- the storage demands to be minimized because of the limited storage capacity
- computation time and computation costs to be minimized.

These criteria are of the greatest importance to the numerical analyst. In this context the question of the existence or uniqueness of the solution is quite often more easily answered than the fulfilment of the requirements listed above.

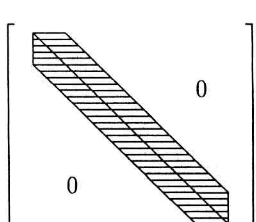
New computer generations allow larger problems to be solved. The VSLI-technology [1] makes it possible to build up highly efficient, economically-priced computers for solving special problems (for example, self-adjoint elliptic partial differential equations).

Examples
There is no exact definition of a sparse matrix. A $(n \times n)$ matrix $A := [a_{ik}]$ is said to be a *sparse matrix* if only a small percentage of all matrix elements a_{ik}, $i, k = 1, 2, \ldots, n$, is nonzero (in practice less than 10%).

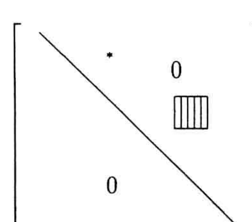
For example, in circuit design the following structures can be found:



Other possible structures are:

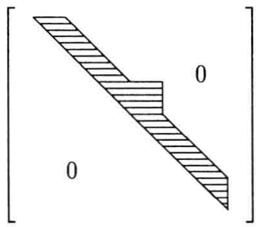


matrix with constant band width

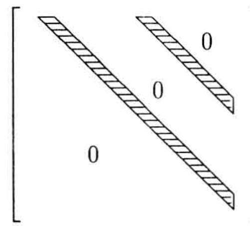


arbitrary sparse matrix

[1] VSLI: Very Large Scale Integrated

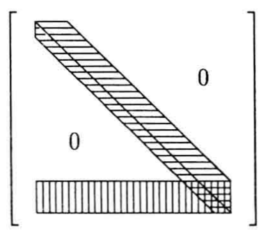


band matrix with step

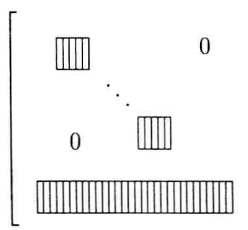


strip matrix

Condensed forms are desirable like:



band matrix with margin



block diagonal matrix with margin

In general it has to be noted that every numerical problem involving sparse matrices must be treated individually; *adaptive algorithms* must be developed.

For example, in continuum mechanics the generalized form of the Poisson equation on a 2-dimensional domain $\mathcal{B}$

$$-\frac{\partial}{\partial x}(a \cdot \frac{\partial u}{\partial x}) - \frac{\partial}{\partial y}(c \cdot \frac{\partial u}{\partial y}) + k \cdot u = f, \quad (x,y) \in \mathcal{B} \subset I\!R^2 \tag{1.1}$$

with $a = a(x,y) > 0, \ c = c(x,y) > 0$ and the boundary conditions

$$\alpha u + \frac{\partial u}{\partial n} = \beta, \ (x,y) \in \Gamma \tag{1.2}$$

has to be solved.

Γ :	closed boundary of $\mathcal{B}$
n :	direction of the normal derivation
α, β :	piecewise continuous function on Γ.

Let $u = u(x, y)$ be a solution and k, f functions continuous within $\mathcal{B}$. In the method of finite elements $\mathcal{B}$ is partitioned into subdomains having forms such as triangles, rectangles and others, shown in Fig.1.1.

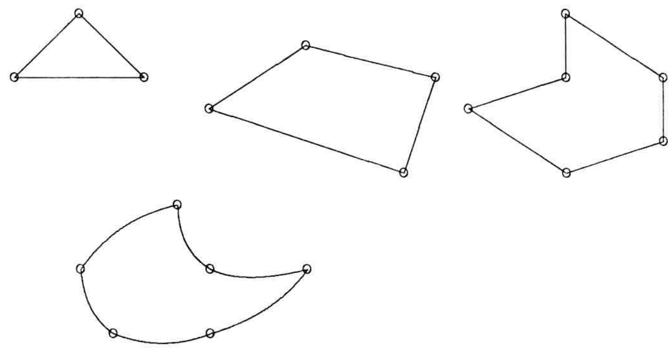


Fig. 1.1 – Examples for partitioned elements

The approximate solution $\hat{u}$ is a polynomial defined on each subdomain of $\mathcal{B}$ fulfilling certain boundary conditions. Finally triangularization of $\mathcal{B}$ leads to the problem of determining the minimal solution $\hat{u}$ of the algebraic equation

$$I(\hat{u}) = \frac{1}{2}(\hat{u}^T A\hat{u} - 2\hat{u}^T b), \tag{1.3}$$

i.e. the system

$$\frac{\partial I}{\partial \hat{u}} = 0 \quad \Leftrightarrow \quad A\hat{u} = b \tag{1.4}$$

has to be solved. The matrix A in this example is of large order, sparse, positive definite and symmetric.

2 Storage techniques

The effectiveness of work with sparse matrices depends not only on the underlying mathematics, but also on the extent to which the computer itself is an integral part of the algorithm. Thus storage techniques play an important role; their aim is to store information as densely and as economically as possible.

Example 2.1
In the frequency analysis of linear networks the linear systems $A(\omega_i)x = b$ have to be solved for different frequencies ω_i. A is Hermitian of order $n = 3304$ with 60685 nonzero elements; hence the density (i.e. the quotient of the number of nonzero elements and the total number of matrix elements) is 0.6 %. *LU*-factorization gives 105470 nonzero elements with a fill-in of 0.4 %. Conventional storage techniques would require about 20 million storage cells.

This example shows some of the properties which storage techniques must possess:

- only nonzero elements should be stored
- it should be possible to insert additionally created nonzero elements easily and quickly into the existing list of nonzero elements.

The treatment of sparse problems is affected considerably by the configuration of the computer available, i.e. according to their importance within the algorithms the data are stored either in fast-working and therefore expensive storages (for example core) or in slower peripheral storage (for example discs). At present various storage modules are available for users in medium-sized and larger equipment.

If an unstructured matrix is sufficiently sparse it can of course be kept throughout in the high-speed storage of a computer: only the elements $a_{ik} \neq 0$ are stored. The placement scheme for these elements in the store depends on the algorithm that needs these elements. Different kinds of storage are available. If the large matrix to be stored is of high density, or the number of nonzero elements exceeds the capacity of the core or high-speed storage, the matrix has to be kept in the low-speed external store and the matrix elements have to be transported in blocks into the high-speed storage. In this context the reader is recommended to study carefully the analysis of paging strategies for the solution of linear systems.

2.1 Linked lists

Each element $a_{ik} \neq 0$ in the column k is stored as an *item* I with

$$I := (i, v, p) \tag{2.2}$$

and

i : row index
v : value of the element a_{ik}
p : address of the next element $a_{ik} \neq 0$ of column k.

The address p is zero, if a_{ik} is the last nonzero element in the column k. Then an item can be depicted as follows:

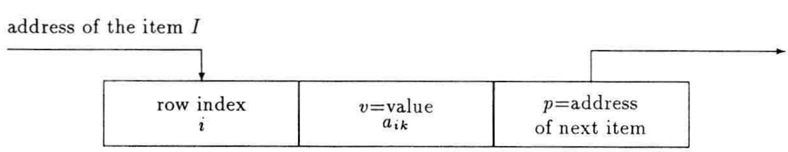


Fig. 2.1 – Item

Besides this block SI of store for the items a further block is needed to store the first address of each column:

BC : beginning of column address

Thus the total storage requirement S consists of both the part BC and part SI. Part BC has exactly n locations and SI requires exactly $3t$ storage locations, where t denotes the number of nonzero elements. The total length of S is: $n+3t$.

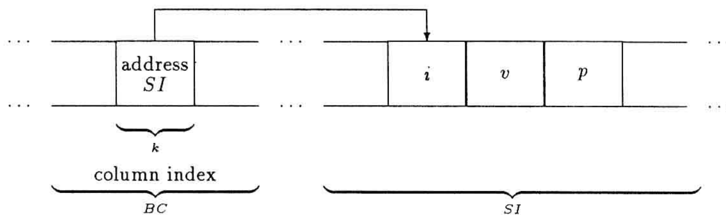


Fig. 2.2 – Total list

In consequence of this storage scheme additionally created nonzero elements can be stored in SI without having to rearrange them. To show how the creation of a new nonzero element affects BC and SI the following example is given:

Example 2.3

$$a_{13} := a_{33} = 0, \ a_{23} := 0.5, \ a_{43} := 1.5.$$

BS begins at location 101, and the items corresponding to a_{23} and a_{43} begin at locations 200 and 203 respectively; the element $a_{33} := 2.5$ is inserted later. This item starts at 300:

Table 2.1 Example

location	101	200	201	202	203	204	205	300	301	302
present contents	200	2	0.5	203	4	1.5	0	-	-	-
new contents	200	2	0.5	300	4	1.5	0	3	2.5	203
	from BS		item $\hat{=} a_{23}$			item $\hat{=} a_{43}$			item $\hat{=} a_{33}$	

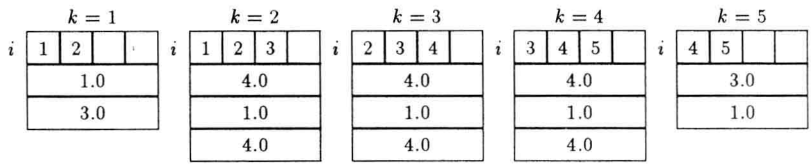
2.2 Storage technique in case of identical matrix elements

The values of the nonzero elements of a sparse matrix often are equal. In this case numerical constants are used. For illustration the following example is given:

Example 2.4
A $(5,5)$-sparse matrix A containing 13 nonzero elements is to be stored by columns.

$$A = \begin{bmatrix} 1.0 & 4.0 & 0 & 0 & 0 \\ 3.0 & 1.0 & 4.0 & 0 & 0 \\ 0 & 4.0 & 1.0 & 4.0 & 0 \\ 0 & 0 & 4.0 & 1.0 & 3.0 \\ 0 & 0 & 0 & 4.0 & 1.0 \end{bmatrix}$$

Usual storage technique yields the following diagram:



k column index, i row index

Fig. 2.3 – Usual storage technique

Since many values of the matrix A are equal a list of the different values is constructed and to each row index is assigned an index of the list of values.

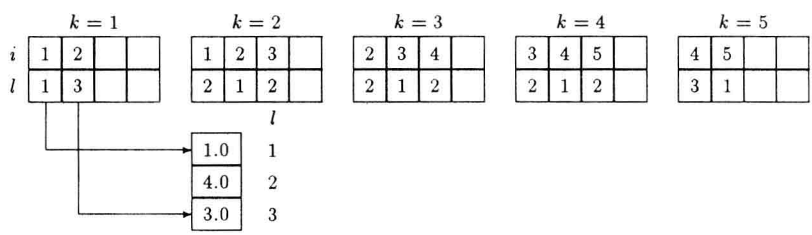


Fig. 2.4 – Modified storage technique

The saving of storage cells may be practically enormous, if, as in a linear programming example, 97000 nonzero elements assume only 4500 different values.

2.3 Unlinked lists

In general unlinked lists need even less storage cells than the techniques described above. These storage techniques are applied to avoid the use of external storages for the matrix elements, since the transportation from the external to the internal storage takes a lot of time. Additionally created nonzero elements (in various steps of the computations) are introduced by *relocating*.

Scheme 2.5
To each nonzero element correspond 2 storage cells containing the row index i and the value a_{ik}. Moreover there are items representing the current column k.

$i = 0$ denotes the end of the current column

An item | 0 | 0 | denotes the end of the matrix storage.