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0521818281 - Iterative Krylov Methods for Large Linear Systems

Henk A. van der Vorst

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Computational simulation of scientific phenomena and engineering problems often depend on solving linear systems with a large number of unknowns. This book gives an insight into the construction of iterative methods for the solution of such systems and helps the reader to select the best solver for a given classes of problems.

The emphasis is on the main ideas and how they have led to efficient solvers such as CG, GMRES, and Bi-CGSTAB. The book also explains the main concepts behind the construction of preconditioners. The reader is encouraged to build his own experience by analysing numerous examples that illustrate how best to exploit the methods. The book also hints at many open problems and, as such, it will appeal to established researchers. There are many exercises that clarify the material and help students to understand the essential steps in the analysis and construction of algorithms.

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Henk A. van der Vorst
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Preface

In 1991 I was invited by Philippe Toint to give a presentation, on Conjugate Gradients and related iterative methods, at the university of Namur (Belgium). I had prepared a few hand-written notes to guide myself through an old-fashioned presentation with blackboard and chalk. Some listeners asked for a copy of the notes and afterwards I heard from Philippe that they had been quite instructive for his students. This motivated me to work them out in $\text{\LaTeX}$ and that led to the first seven or so pages of my lecture notes. I took the habit of expanding them before and after new lectures and after I had read new interesting aspects of iterative methods. Around 1995 I put the then about thirty pages on my website. They turned out to be quite popular and I received many suggestions for improvement and expansion, most of them by e-mail from various people: novices in the area, students, experts in this field, and users from other fields and industry.

For instance, research groups at Philips Eindhoven used the text for their understanding of iterative methods and they sometimes asked me to comment on certain novel ideas that they had heard of at conferences or picked up from literature. This led, amongst others, to sections on GPBi-CG, and symmetric complex systems. Discussions with colleagues about new developments inspired me to comment on these in my Lecture Notes and so I wrote sections on Simple GMRES and on the superlinear convergence of Conjugate Gradients.

A couple of years ago, I started to use these Lecture Notes as material for undergraduate teaching in Utrecht and I found it helpful to include some exercises in the text. Eventually, the text grew larger and larger and it resulted in this book.

The history of the text explains more or less what makes this book different from various other books. It contains, of course, the basic material and the required theory. The mathematical presentation is very lecture inspired in the

sense that I seldom prove theorems in lectures: I rather present the successive ideas in a way that appears logical, at least to me. My presentation of the Bi-CG method is an example of this. Bi-CG can be presented in a very short and clean way once the method is known. However, I preferred to introduce the method from the point of view of the person who only knows CG and has learned that CG does not work for unsymmetric systems. The natural question then is how to repair the method, retaining its short recurrences, so that unsymmetric problems can be solved. This is exemplary for the major part of the text. In most cases I try to present the ideas in the way they may come up in a discovery phase and then I, sometimes, collect interesting conclusions in theorems. I only included in some cases a more formal ('afterward') proof.

The text contains the basic material for the best known iterative methods and most of them are shown in frames in a way that facilitates implementation in Matlab. The experiments have been carried out with my own Matlab versions of the framed algorithms. The experiments are also rather unusual. They are very simple and easy to repeat. They are of a kind that anyone can come up with rather quickly. However, by inspecting the behaviour of the various methods for these simple problems, we observe various aspects that are typical for the more complicated real-life problems as well. I have seen many large and complicated linear systems and I have advised researchers in the industry on how to solve these systems. I found it always instructive to explain expected effects with the help of very simple small examples. I expect that these experiments and the discussions will add more life to the material for industrial users and that they will help students to construct other, even more interesting, test examples. I hope too that my discussions will stimulate students to discover other new aspects and to think about these.

Apart from the basic material, the text focuses on aspects that I found particularly interesting. Mostly these are aspects that lead to more insight or to better methods, but sometimes I have also included discussions on ideas (of others), which have less certain outcomes. Hence the book may also be of interest to researchers, because it hints at many avenues for new research.

I know that some of my colleagues have used older versions of this text for teaching, at various levels. For that purpose I have included all sorts of exercises in the text. As a student I did not like many of the exercises that we had to do, which served as tests afterwards. I preferred exercises that helped me understand the text when I needed it most. With this in mind I have constructed the exercises. In most cases they concern essential parts of the presentation and they are placed in the text where their results are most helpful for deeper understanding. Often I refer to results and formulas obtained in these exercises. Other exercises are intended to motivate students to construct working examples

and to teach them to draw, and sometimes prove, correct conclusions. These exercises can be made with the help of short Matlab, or Mathematica, codes that the students have to write themselves, guided by the framed algorithms. Some of the problems can also be handled with the existing Template codes for various Krylov subspace methods, including CG, Bi-CG, GMRES, CGS, QMR, and Bi-CGSTAB. These methods are standard and are available in Matlab 6.0 and more recent versions. They are also available through the Web at the famous netlib website.

This is the place to thank numerous colleagues for their suggestions and comments. Over the past ten years they have been so numerous that it is impossible to mention all of them and it would also be unfair not to mention the many persons from various audiences that helped me, through their questions and comments, to improve my presentation of the material. I would like to make a few exceptions. I am particularly indebted to Michael Saunders, who helped me to correct part of the text while we were at a workshop in Copenhagen. I also learned very much about the subject from collaborations with Iain Duff, Gene Golub, and Youcef Saad, with whom I wrote a number of overview papers. These were extremely pleasant and fruitful events.

Dear reader of this book, I hope very much that this text will be helpful to you and I would appreciate hearing your comments and suggestions for further improvement.

Henk van der Vorst