ITERATIVE PROJECTION METHODS FOR SPARSE LINEAR SYSTEMS AND EIGENPROBLEMS
CHAPTER 1 : INTRODUCTION

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Introduction

Two fundamental tasks in numerical computing are the solution of a linear system of equations

$$Ax = b$$

where $A \in \mathbb{R}^{n\times n}$ and $b \in \mathbb{R}^n$ are given, and the solution of linear eigenvalue problems

$$Ax = \lambda x \quad \text{or} \quad Ax = \lambda Bx$$

.

These systems arise very frequently from finite element or finite volume or finite difference approximations to boundary value problems and the dimension n of the problem can be very large. $n = 10^5$ to $n = 10^6$ are not unusual.

Example

Consider the boundary value problem

$$\left.\begin{aligned} -\Delta u = f\,, \quad & \text{in} \quad \Omega := \{(x,y,z)^T \in \mathbb{R}^3 \,:\, 0 \le x,y,z \le 1\} \\ u = g\,, \quad & \text{on} \quad \partial\Omega. \end{aligned}\right\}$$

If we discretize the differential equation employing central differences

$$\begin{aligned} \Delta u(x,y,z) \approx \frac{-1}{h^2}\Big(& 6u(x,y,z) - u(x+h,y,z) - u(x-h,y,z) \\ & -u(x,y+h,z) - u(x,y-h,z) - u(x,y,z+h) - u(x,y,z-h)\Big) \end{aligned}$$

then we obtain for $h := 1/(m+1)$ the following system of linear equations

Discretization by finite differences

$$\begin{aligned} &6U_{i,j,k} - U_{i-1,j,k} - U_{i+1,j,k} - U_{i,j-1,k} - U_{i,j+1,k} - U_{i,j,k-1} - U_{i,j,k+1} \\ &\quad = h^2 f(ih, jh, kh), \quad i,j,k = 1,\ldots,m, \end{aligned} \tag{1}$$

where $U_{i,j,k}$ denotes an approximation to $u(ih, jh, kh)$ for $i,j,k = 1,\ldots,m$ and $U_{i,j,k} = g(ih, jh, kh)$ if $i \in \{0, m+1\}$ or $j \in \{0, m+1\}$ or $k \in \{0, m+1\}$.

For the moderate step size $h = 1/101$ the dimension of the system is already $n = 10^6$.

Notice however that the matrix of the system is sparse, i.e. most of the entries are 0.

Solution of large linear systems

There are essentially two approaches to the numerical solution of large and sparse linear systems.

- One is to adapt direct methods, such as Gaussian elimination (which obtain the solution of the system in a finite number of operations), to exploit the sparsity structure of the system matrix A. Typical adaption strategies involve the intelligent choice of the numbering of the unknowns (to minimize the band width of the matrix or to obtain special data structures) or special pivoting rules to minimize fill-in in the elimination process. We are not going to study these methods in this course.
- Most of the methods in use today for large and sparse linear systems are iterative. These methods try to improve an initial approximation x^0 of the solution by generating a sequence of approximate solutions x^k, $k = 1, 2, \ldots$, of (hopefully) increasing accuracy.

Advantages of iterative solvers

upon direct methods are the following ones

- The system matrix A is not needed in explicit form but only a procedure to compute the matrix-vector product Ax for a given vector $x \in \mathbb{R}^n$. This is especially advantageous in finite element applications where the product Ax can be performed elementwise.
- Preinformation about the solution which usually is at hand in engineering applications can be introduced into the solution process via the initial approximation x^0.
- Usually, the linear system under consideration is the discrete version of a system with an infinite number of degrees of freedom (which itself is only a model of the real system). Hence, it does not make any sense to compute the solution of the linear system with higher accuracy than the discretization error. Iterative methods can be terminated when the desired accuracy is derived. Hence, they require only the employment of those resources (time, memory) which are necessary to obtain the wanted accuracy.

direct vs. iterative solution

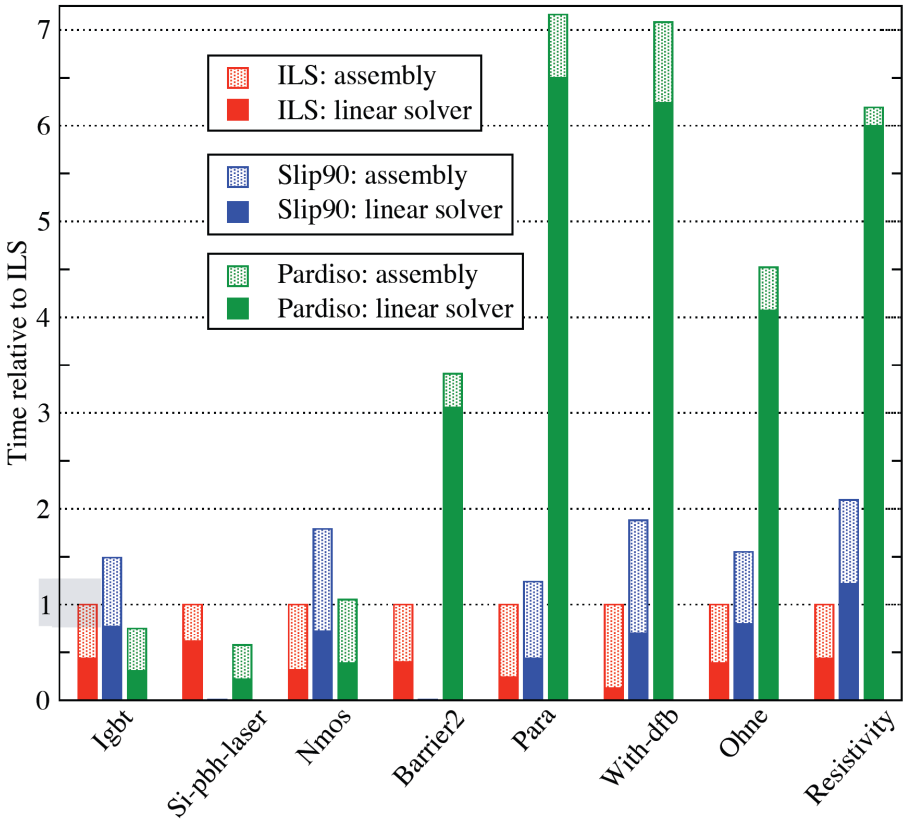
An example: semiconductor device simulation (thanks to Martin Gutknecht, ETH Zürich)

Collection of test matrices arising in semiconductor device simulation:

Name	n	# nonzeros	space dimension
Igbt-10	11 010	234 984	2D
Si-pbh-laser-21	14 086	511 484	2D
Nmos-10	18 627	387 457	2D
Barrier2-7	115 625	6 372 663	3D
Para-7	155 924	8 374 204	3D
With-dfb-36	174 272	8 625 700	3D
Ohne-9	183 038	11 170 886	3D
Resistivity-9	318 026	19 455 650	3D

direct vs. iterative solution

Compare performance of 3 state-of-the-art computer codes



ILS, Slip90: iterative solvers based on BiCGStab

PARDISO: sparse direct solver

Historical remark

The idea of solving linear systems by iterative methods dates back at least to Carl Friedrich Gauß roughly 180 years ago. The method of least squares yielded systems which were too large to be handled by elimination methods if someone used only pencil and paper.

In his paper “Supplementum theoriae combinationis observationum erroribus minimae obnoxiae” (1819 - 1822) Gauß described an iteration method which is called block-Gauß-Seidel-method today. He was so fascinated by this method that he wrote in a letter to Gerling in 1823

> *“Ich empfehle Ihnen diesen Modus zur Nachahmung. Schwerlich werden Sie je wieder direkt eliminieren, wenigstens nicht, wenn Sie mehr als 2 Unbekannte haben. Das indirekte Verfahren lässt sich halb im Schlafe ausführen, oder man kann während desselben an andere Dinge denken.”*

In English: “I recommend this method for imitation. Hardly you will ever again eliminate directly, at least not if the system has more than two unknowns. The indirect method can be performed half in sleep or you can think about other things at the same time.”

Historical remark ct.

Methods which are quite similar to that of Gauß were described by Carl Gustav Jacobi in 1845 and Phillip Ludwig Seidel in 1874.

Since the emergence of digital computers the dimension of systems that could be treated numerically grew enormously. It turned out that the convergence of classical methods is far too slow for discrete versions of boundary value problems for partial differential equations. A substantial improvement was derived at the end of the forties of the last century by relaxation methods which were introduced by Southwell and Young.

In 1952 Hestenes and Stiefel independently developed the conjugate gradient method which, in exact arithmetic, is a direct method (i.e. it generates the exact solution in a finite and predetermined number of operations). It was soon realized that round off errors destroy this finite convergence property and that the method was not an efficient alternative to factorization for dense systems.

Historical remark ct.

Stiefel, Rutishauser and others already discussed the iterative aspects of the conjugate gradient method for discrete versions of boundary value problems at the end of the fifties.

A revival of the method as an iterative procedure was initiated by the work of Reid at the beginning of the seventies of the last century, who observed that for certain large problems sufficiently good approximations were obtained in far less steps than are needed to get the exact solution.

Today, together with its numerous variants, it is the standard method for the numerical treatment of large and sparse linear systems, especially when preconditioning is used.

In the first half of this summer school we survey this type of iterative methods for linear systems.

Eigenvalue problems

Generalizations of the conjugate gradient methods are iterative projection methods where the system under consideration is projected to a space of small dimension called search space.

If one is not yet satisfied with the accuracy of the approximate solution, then the search space is expanded by some vector, and this expansion is repeated until (hopefully) convergence.

Solvers for sparse eigenvalue problems follow the same lines, and they have many properties in common with solvers of linear systems.

Two types of iterative projection methods for eigenproblems are considered in this summer school; methods which projected the underlying problem to a sequence of Krylov spaces, and methods, where the search space is expanded by a direction which has a high approximation potential for the eigenvector wanted next.

Nonlinear eigenvalue problems

In the last section of the summer school we consider generalizations of iterative projection methods to nonlinear eigenvalue problems, i.e.

If $T(\lambda) \in \mathbb{C}^{n\times n}$, $\lambda \in D \subset \mathbb{C}$ is a family of matrices, then $\lambda \in D$ is an eigenvalue and $x \neq 0$ is a corresponding eigenvector, if

$$T(\lambda)x = 0.$$

Problems of this type arise in vibrations of conservative gyroscopic systems, damped vibrations of structures, problems with retarded argument, lateral buckling problems, fluid-solid vibrations, quantum dot heterostructures, and sandwich plates, e.g.

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