

Lecture 1

Introduction to Iterative and Multigrid Methods

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About the Course

- The book: "Iterative Methods for Sparse Linear Systems" Second Edition by Yousef Saad.



- 1st vs 2nd: mutligrid and domain decomposition chapters, improved homework sets, improved readability
- Course requirements: CS450
- Course knowledge: programming, basic linear algebra, some numerical PDEs

Assessment

- read/discuss a few technical papers
- HW's are generally bi-weekly:
 - collection of book problems and homemade
 - code: C,C++,Matlab
 - ★ can “follow” existing packages, but should be your own writing
 - ★ maintain a consistent library of routines throughout the semester
- Two projects
 - ① Krlyov project (shorter “midterm”)
 - ② MG project (“final”)
- Participation grade: volunteer for a 5-10 minute overview talk. They will come up during the lectures; prepare for the next lecture (low prep).

Assessment

tentative

Homework	40%
Midterm Project	20%
Final Project	30%
Participation	10%



Assessment

First Test: email lukeo the following: (Subject: cs550)

- email address
- C proficiency: 1 to 5
- C++ proficiency: 1 to 5
- Matlab proficiency: 1 to 5
- Python proficiency: 1 to 5
- T/F I have implemented CG
- T/F I have implemented GMRES
- T/F I have implemented AMG

Proficiency: 1==no clue, 2==can read, 3==can pick it up quickly if needed, 4==pretty good, your goto language, 5==h4x0r



Lots of Software

- Bebop
- blitz
- boost
- CSpase
- ITSOL
- Meschach
- MTL
- SPARSEKIT
- sparselib
- splib
- TNT
- many, many, many more

Need a short overview of currently available sparse matrix packages and converters. Any takers?



Topics Overview

- 1/6 Introduction
 - ▶ all things matrixy
 - ▶ some background on iterative and multigrid methods
 - ▶ data structures, sparse BLAS, reorderings, etc
 - ▶ numerical PDEs
- 2/6 Krylov Methods
 - ▶ Basic Methods (Jacobi, GS, SSOR)
 - ▶ A projection approach (SD, MR)
 - ▶ Krylov Taxonomy:
 - ★ Arnoldi: FOM, GMRES
 - ★ Lanczos: CG
 - ★ Faber-Manteuffel roadblock
 - ★ Extending: biorthogonality (BiCG, QMR)
 - ★ Extending: transpose-free (BiCGstab, CGS, TFQMR)



Topics Overview

- 1/6 Preconditioning
 - ▶ big idea
 - ▶ PCG, PGMRES efficient algorithms
 - ▶ Jacobi, ILU, SPAI
- 2/6 Multigrid
 - ▶ 25% Geometric MG with Fourier analysis (book)
 - ▶ 75% algebraic MG (extra notes)
 - ▶ RS AMG
 - ▶ SA AMG time permitting
 - ▶ final project will be AMG based
 - ▶ most likely a code contest
- 0/6 Parallel
 - ▶ will be a project option
 - ▶ mostly algorithmic details
 - ▶ more in CS554



Course Goals

- To obtain working knowledge of sparse matrices
- To build intuition of Krylov methods from a projection approach
- To build intuition of Krylov methods an efficiency perspective
- To construct a working collection of solvers
- To develop an understanding of multigrid to a research level
- To establish a practical understanding of iterative and multigrid methods

What we do

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- Solve *sparse* linear systems $Ax = b$ (and eigenvalue problems $Av = \lambda v$)
- Sparse matrices: matrices that contain mostly zero entries, reducing storage (more later)
- Applications *everywhere*...
- ... more applications *everywhere*



Some history

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Sparse matrices have been identified as important early on — origins of terminology is quite old. Gauss defined the first method for such systems in 1823 (now the Gauss- Seidel iteration). Varga used explicitly the term 'sparse' in his 1962 book on iterative methods.

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- Special techniques used for sparse problems coming from Partial Differential Equations
- One has to wait until to the 1960s to see the birth of the general technology available today
- Graphs introduced as tools for Sparse Gaussian matrices in 1961 [Seymour Parter]
- Early work on reordering for banded systems, envelope methods



Some history

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- Various reordering techniques for general sparse matrices introduced.
- Minimal degree ordering [Markowitz - 1957] ...
- ... later used in Harwell MA28 code [Duff] - released in 1977.
- Tinney-Walker Minimal degree ordering for power systems [1967]
- Nested Dissection [A. George, 1973]
- SPARSPAK [commercial code, Waterloo]
- Elimination tree, symbolic factorization, ...



Iterative Methods: A history

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- 1950s up to 1970s : focus on “relaxation” methods
- Development of ‘modern’ iterative methods took off in the mid-70s. but...
- ... The main ingredients were in place in 1951-1952 [Lanczos; Arnoldi ; Hestenes (a local!) and Stiefel;]
- The next big “discovery” was that of preconditioning: in effect a way of combining iterative and (approximate) direct methods — [Meijerink and Van der Vorst, 1977]



Eigenvalue Problems: A history

- Another parallel branch was followed in solution methods for large eigenvalue problems.
- in the 1950s and 1960s a big problem was that of utter of airplane wings.. This leads to a large (sparse) eigenvalue problem
- The same methods for linear systems can be extended to eigenvalue problems [Lanczos, Arnoldi]



Matrix Resources

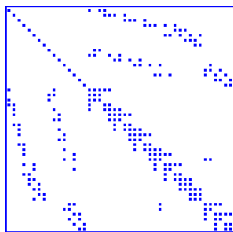
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- Matrix Market: <http://math.nist.gov/MatrixMarket/>
- Florida collection:
<http://www.cise.u.edu/research/sparse/matrices/>
- FE Market: <http://www.cs.berkeley.edu/madams/femarket>
- SPARSEKIT (Saad): <http://www.cs.umn.edu/saad/software>



Sparse Matrices

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- Vague definition: matrix with few nonzero entries
- For all practical purposes: an $m \times n$ matrix is sparse if it has $\mathcal{O}(\min(m, n))$ nonzero entries.
- This means roughly a constant number of nonzero entries per row and column



Sparse Matrices

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- Other definitions use a slow growth of nonzero entries with respect to n or m .
- Wilkinson's Definition: “..matrices that allow special techniques to take advantage of the large number of zero elements.” (J. Wilkinson)”
- A few applications which lead to sparse matrices: Structural Engineering, Computational Fluid Dynamics, Reservoir simulation, Electrical Networks, optimization, Google Page rank, information retrieval (LSI), circuit simulation, device simulation,



Sparse Matrices: The Goal

- To perform standard matrix computations economically i.e., without storing the zeros of the matrix.
- For typical Finite Element /Finite difference matrices, number of nonzero elements is $\mathcal{O}(n)$.

Example

To add two square dense matrices of size n requires $\mathcal{O}(n^2)$ operations. To add two sparse matrices A and B requires $\mathcal{O}(nnz(A) + nnz(B))$ where $nnz(X)$ = number of nonzero elements of a matrix X .

remark

A^{-1} is usually dense, but L and U in the LU factorization may be reasonably sparse (if a good technique is used).



Next Time

- Sparse Matrices: Data structures
- Sparse Matrices: graph
- Sparse Matrices: reorderings
- FE/FD
- Read §1.1-1.5
- First HW out on Thursday
- remember to email me

