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ITERATIVE METHODS FOR SOLVING LINEAR SYSTEMS

Lecture 3. Krylov subspace iterative methods

Nizhni Novgorod

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OBJECTIVES

The objective of this lecture is to review a general approach to construction of Krylov subspace iterative methods. The generalized minimum residual method, conjugate gradient method and biconjugate gradient method are used as examples. The lecture also reviews preconditioning for the above algorithms.

ABSTRACT

This lecture is dedicated to iterative methods based on Krylov subspaces. These methods are used to solve $Ax=b$ linear systems. It is understood that the matrix A remains unchanged in the course of solving and the most complex operation that may be used is multiplying the matrix by a vector, i.e. determining $y=Ax$ for the given x.

There are numerous methods based on Krylov subspaces. Some of them are suitable for nonsymmetric matrices, while others require a symmetric or a positive definite matrix. Some of methods for nonsymmetric matrices allow not only for products like Ax, but also for $A^T x$-type products. In this lecture we will review three typical methods. They are the generalized minimum residual (GMRes) method, biconjugate gradient (BiCG) method and conjugate gradient (CG) method. Preconditioning will be considered for all the methods above.

GUIDELINES

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There are numerous methods based on Krylov subspaces. Some of them are suitable for nonsymmetric matrices, while others require a symmetric or a positive definite matrix. Some of methods for nonsymmetric matrices allow not only for products like Ax, but also for $A^T x$-type products. As part of this lecture, we will review three typical methods. They are the generalized minimum residual (GMRes) method, biconjugate gradient (BiCG) method and conjugate gradient (CG) method. Preconditioning will be considered for all the methods above.

The first part of this lecture will introduce essential concepts related to Krylov subspaces. We will define the subspace $K_m(A,v)$ with the dimension m, produced by the vector v and matrix A.

We will also set the problem of finding the basis $\{v_1, v_2, \ldots, v_m\}$ of a Krylov subspace. To solve it, we will formulate the Arnoldi's algorithm to construct the orthonormal subspace basis. The algorithm complexity characteristics will be listed. We will also set the related task of construction of two biorthogonal bases $\{v_1, v_2, ..., v_m\}$ and $\{w_1, w_2, ..., w_m\}$ for the subspaces $K_m(A, v_1)$ and $K_m(A^T, w_1)$. To solve it, we will formulate the Lanczos algorithm. The lecture will demonstrate that the Lanczos algorithm is much less complex compared to the Arnoldi's algorithm. The two algorithms above serve as a basis of computational procedures for Krylov subspace iterative methods.

The next part of this lecture will deal with the generalized minimum residual (GMRes) method. This method is intended to solve linear systems with a $n \times n$ nonsingular matrix A (unlike the basic iterative methods studied earlier, this method may be applicable to nonsymmetric and indefinite matrices). The generalized minimum residual (GMRes) method has the following idea. Let us consider a Krylov subsystem K_m constructed using a normalized residual vector $v = r_0 / \| r_0 \|$ of the initial approximation x_0. The generalized minimum residual approximates the exact linear system solution x^* by the vector x_m from the subspace $x_0 + K_m$. For this purpose, the least-squares problem is solved at each method iteration, being restricted to solving the auxiliary linear system with a $m \times m$ dense matrix, where m is the iteration number. The GMRes algorithm guarantees (without round-off errors) convergence to the exact problem solution for maximum n iterations, where n is the matrix A dimension.

As it appears from the algorithm description, its implementation requires storage of an $m \times m$ auxiliary system matrix and a $n \times m$ basis vector matrix of the Krylov subsystem (here, m is the Krylov subspace dimension and n is the matrix A dimension). Therefore, as m increases, overheads for both basis vector matrix storage and auxiliary linear system solution grow. To work it around, it is recommended to restart the method from the current approximation. In order to improve the convergence rate of GMRes и GMRes(m), a preconditioning is introduced. The lecture lists the result of computational experiments that prove reduction of the number of iterations in case of preconditioning.

The third part of this lecture will deal with the biconjugate gradient (BiCG) method. Similar to GMRes, BiCG is intended for linear systems with a $n \times n$ nonsingular matrix A. At the same time, unlike GMRes, BiCG requires less memory but computes products expressed as $A^T x$ which ensures efficient access to the matrix A columns.

The biconjugate gradient method is based on the Lanczos biorthogonalization (just like the conjugate gradient method is based on the Lanczos symmetric ortogonalization). The implicitly described method not only solves the initial problem $Ax = b$, but also the dual system $A^T \bar{x} = \bar{b}$. The method is based on the property of bi-conjugacy (or just conjugacy if the matrix A is clear from the context) of the two vector systems, $\{p_1, ..., p_m\}$ and $\{\bar{p}_1, ..., \bar{p}_m\}$. Bi-conjugacy is equivalent to biorthogonality for the scalar *A*-product, therefore, to find the vector systems $\{p_1,..., p_m\}$ and $\{\overline{p}_1,..., \overline{p}_m\}$, the Lanczos algoritm with the scalar *A*-products may be used. Then we will formulate the bi-conjugate gradient method and see how the preconditioner *M* is used within its computation scheme. As part of the lecture, we will list experimental results that demonstrate reduction of the number of iterations for the preconditioned BiCG method. Please note that the method uses the matrices A^T and M^T, respectively, so it may be difficult to use it if obtaining transposed matrices is a complex operation due to the character of the solved problem.

The last part of the lecture describes the conjugate gradient (CG) method intended for linear systems with a $n \times n$ symmetric positive definite matrix *A*. All the Krylov subspace iterative methods cited above do not assume any additional properties of the matrix A, so they can be applied directly to a system with a symmetric matrix, too. However, provision for symmetry will enable simplification of the BiCG computation scheme which, in its turn, facilitates method implementation and makes the respective requirements to resources more relaxed.

First of all, for a symmetric Krylov subspace matrix, $K_m(r_0, A)$ and $K_m(r_0, A^T)$ will coincide. This means that the BiCG method does not require storage and processing of the conjugate vectors $\overline{r}_i$ and $\overline{p}_i$. In this case, the condition of vector p_i and $\overline{p}_j$ bi-conjugacy transforms to the condition of conjugacy $(Ap_i, p_j) = 0$ when $i \neq j$. This lets us formulate the CG method as a symmetric BiCG version.

It can be shown that finding the exact solution for a linear system with a symmetric positive definite matrix requires no more than *n* iterations, so the complexity of the exact solution search algorithms reaches $O(n^3)$. However, due to round-off errors this process is usually considered iterative; the process is completed when the condition of small relative residual is satisfied.

The preconditioner *M* is introduced into the CG method scheme in a standard way. Let us note once again that the use of preconditioner does not involve calculation of the matrix M^{-1}, but requires solving a system with the matrix *M* at each method iteration. Similar to the methods described earlier, the experimental results demonstrate a significant influence of the preconditioner on the convergence rate of the CG method.

RECOMMENDATIONS FOR STUDENTS

A description of Krylov subspace iterative methods can be found in numerous publications as such methods are the best iterative methods to solve linear systems. See [1] for a concise method description (including pseudocode algorithms). A detailed description of the approach in whole including determination of methods, their theoretical justification and examples of use can be found in [4]. See [2, 3] for a description of the preconditioned conjugate gradient method as a typical Krylov subspace iterative method.

REFERENCES

1. J. Dongarra et al. Templates for the solution of linear systems: building blocks for iterative methods. SIAM, 1994.
2. Gene H. Golub, Charles F. Van Loan. Matrix Computations. The John Hopkins University Press, 1996.
3. James W. Demmel. Applied Numerical Linear Algebra. SIAM, 1997.
4. Y. Saad. Iterative Methods for Sparse Linear Systems. SIAM, 2003.

PRACTICE

1. Implement the GMRes(m) method (generalized minimal residual method with restart). Compare the number of method iterations for various restart parameter *m* values.
2. Implement the BiCG-Stab method (stabilized biconjugate gradient method) using the pseudocode indicated in [1]. Compare convergence rates of the initial and stabilized methods.
3. Use the ILU(0)-preconditioner for the methods from previous tasks. Compare the number of iterations for the initial and preconditioned methods.

TEST

1. What systems are solvable using the generalized minimum residual method?
   a. Only systems witha symmetric positive definite matrix
   b. Only systems with a symmetric matrix
   c. + Systems with a general matrix
2. What systems are solvable using the biconjugate gradient method?
   a. Only systems with a symmetric positive definite matrix
   b. Only systems with a symmetric matrix
   c. + Systems with a general matrix
3. As compared to the GMRes method, the BiCG method
   a. + Requires less free memory to operate
   b. Is less complex
   c. Solves a wider range of problems
4. Can the BiCG method be considered as a direct method of solving linear systems?
   a. + Yes

b. Yes, but only for well-conditioned matrices
c. No

5. How many operations are required to ensure guaranteed convergence of the conjugate gradient method to solve a linear system with a $n \times n$ matrix?
   a. $n/2$
   b. + n
   c. $2n$
6. Which operations are used to construct the Krylov subspace basis for the matrix A?
   a. + Matrix multiplication by a vector
   b. Matrix multiplication by a matrix
   c. Matrix inversion
7. The Arnoldi and Lanczos algorithms
   a. have the same degree of complexity
   b. + the Arnoldi algorithm is more complex
   c. + the Lanczos algorithm is more complex
8. To solve linear systems with a symmetric positive definite matrix, one can use
   a. Conjugate gradient method
   b. Biconjugate gradient method
   c. Generalized minimal residual method
   d. +All the above methods
9. For the GMRes method, the auxiliary linear system to be solved at each iteration, has a
   a. Triangular matrix
   b. + Almost triangular (Hessenberg) matrix
   c. Tridiagonal matrix
10. Use of the preconditioner M in an iterative method involves
    a. Computation of the matrix M^{-1} and transition to the problem with the matrix $M^{-1}A$.
    b. + Solving a system with the matrix M at each method iteration
    c. Solving a system with the matrix M at the first method iteration