COMPARISON OF ITERATIVE METHODS FOR SPARSE LINEAR SYSTEMS

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Abstract

This paper presents comparison of iterative methods for sparse linear systems containing large sparse systems. While direct methods are more in use and are error free, they are often expensive and time consuming. A comparison of some options such as the popular steepest-descent and conjugate gradient method are presented. Other methods such as the Arnoldi iteration are also given.

Key Words :*Linear Systems, Sparse Matrices, Sherman-Morrison, Steepest Descent, Conjugate Gradient, Conjugate Directions, GMRES, Arnoldi iteration.*

3. INTRODUCTION

Linear systems are systems that use linear operators. In this paper, it deals with methods to solve linear systems of the form $Ax = b$ where A is a matrix of coefficients, x is a column vector composed of variables and b is a column vector with the given values.

Even though there are various methods available to solve linear systems such as the Gaussian elimination, LU-factorization method, etc., it can get cumbersome while solving large systems in reality. This paper looks at systems involving sparse matrices.

4. Solving Sparse Linear Systems

There are easier methods than the ones outlind here, to solve linear systems, Cramer's Rule being one of them. However, the implementation of such methods on matrices of high dimensions becomes difficult. Hence, the ones outlined in the following becomes an easier option for solving such systems.

4.1 Sherman-Morrison Formula

The Sherman-Morrison Formula uses the idea of replacing the original matrix in the sum of matrix A and the product of the vectors u and v.

For a linear system $Ax = b$,where the $n \times n$ matrix $A$is a special or an almost special form such as triangular or tridiagonal, the Sherman-Morrison formula can be used to solve the linear system. It provides a formula to find the inverse of a matrix $A = B - uv^t$,where $B$is a nonsingular $n \times n$ matrix.

A is nonsingular if and only if $1 - v^t(B^{-1}u) \neq 0$. In this case, the Sherman Morrison formula is

$$A^{-1} = \left(I + \frac{1}{1 - v^t(B^{-1}u)}(B^{-1}u)v^t\right)B^{-1}$$

From the Sherman-Morrison Formula, the following algorithm can be formed to find the solution for $Ax = b$(MIT, 2006)**:**

i. Solve $Bz = u$.
ii. Find $\alpha = 1 - v^t(B^{-1}u) = 1 - v^t z$
    a. If $\alpha = 0$, A is singular and hence A^{-1} cannot be found.
    b. If $\alpha \neq 0$, A is non singular and A^{-1} exists.
iii. Solve $By = b$.
iv. Find $\beta = \frac{v^t y}{\alpha}$.
v. The solution for $Ax = b$ is $x = y + \alpha z$.

The Sherman-Morrison formula can be applied to a class of sparse problems. This is particularly useful if the inverse of B is provided or can be calculated quickly. It allows the method to build up for more complicated matrices by adding a row or a column at a time. The method is especially useful as a rank-one change in a matrix results in a rank-one change in the

inverse of the matrix. It requires $O(n^2)$ operations to find the inverse in comparison to $O(n^3)$ operations needed by another method such as the Gaussian elimination. While this is suitable for application for rank-one changes. It becomes unstable wit repeated use as the approximation errors grows with the repetitions.

2.2. The Method of Steepest Descent

The steepest descent method is an iterative process and is also known as gradient descent. It uses minimization of f, which is of quadratic form (Boyd, 2008)(Shewchuk, 1994):

$$f(x) = \frac{1}{2}x^T Ax - b^T x + c$$

where A is symmetric and positive definite, x and b are vectors and c is a scalar constant. $f(x)$ is minimized by the solution to the system $Ax = b$. In this method, it starts off with $x_i, i = 0$

$$x_{i+1} = x_i + \alpha_i r_i$$

α needs to be found to minized the function and the following definitions can be used:

The residual: $r_i = b - Ax_i, r_{i+1} = b - Ax_{i+1}$

The error: $e_i = x_i - x$

And $r_i = -Ae_i = -f'(x)$. We have $r_{i+1}^T r_i = 0$, and according to the above definitions:

$$(b - Ax_{i+1})^T r_i = r_i\big(b - A(x_i + \alpha_i r_i)\big)^T$$
$$(b - Ax_i)^T r_i = \alpha(Ar_i)^T r_i$$

Using $A = A^T$

$$r_i^T r_i = \alpha r_i^T (Ar_i)$$
$$\alpha = \frac{r_i^T r_i}{r_i^T Ar_i}$$

2.3 The Method of Conjugate Directions (CD)

This method involves taking one step in each search direction and choosing a point x

$$x_{i+1} = x_i + \alpha_i d_i,$$

which gives

$$e_{i+1} = e_i + \alpha_i d_i.$$

For finding α_i, e_{i+1} must be orthogonal to the directions $d_0, d_1, \dots, d_i$.

Here, $d_i^T e_{i+1} = 0, d_i(e_i + \alpha_i d_i) = 0$, thus

$$\alpha_i = \frac{(-d_i^T e_i)}{d_i^T d_i}$$

If d_i and d_j to be conjugate, then $d_i^T Ad_j = 0$, where A is symmetric matrix. When the search directions are A-orthogonal

$$\alpha_i = \frac{-d_i^T Ae_i}{d_i^T Ad_i}$$

As $-Ae_i = r_i$

$$\alpha_i = \frac{d_i^T r_i}{d_i^T Ad_i}$$

The error term is

$$e_i = e_i + \sum \alpha_j d_j$$

2.4 Method of Gram-Schmidt Conjugation

This method is used to find minimum point of quadratic functions. By setting $u_i = d_i$ for $i > 0$ and using the definition of error term in the method of CD,

$$d_i = u_i + \sum B_{ik} d_k$$

Premultiplying this equation by Ad_j, we have

$$d_i^T Ad_j = u_i^T Ad_j + \sum B_{ik} d_k^T Ad_j$$
$$B_{ik} = \frac{-u_i^T Ad_j}{d_j^T Ad_j}$$

2.5 Conjugate Gradient

Conjugate gradient (CG) method is an iterative method to solve large systems of linear equations involving large sparse systems.

The algorithm can be summarized as:

i. An approximated initial solution can be the input vector x_i for $i = 0$.
$$d_i = r_i, r_i = b - Ax_i$$

ii. From steepest descent method, the scalar α_i can be computed
$$\alpha_i = \frac{r_i^T r_i}{d_i^T Ad_i}$$

iii. Find
$$x_{i+1} = x_i + \alpha_i d_i$$

iv. Compute next residual vector
$$r_{i+1} = r_i - \alpha_i Ad_i$$

v. From CD and gram-schmidt method find scalar
$$\beta_{i+1} = \frac{r_{i+1}^T r_{i+1}}{r_i^T r_i}$$

vi. Using the scalar β, obtain next search direction
$$d_{i+1} = r_{i+1} + \beta_{i+1} d_i$$
and repeat for $i = i + 1$. Result is x_{i+1}.

2.8 Arnoldi Iteration

This method can be used on linear systems and eigenvalue problems. A general, nonsymmetric A is

reduced to a Hessenberg form.

Let Q_n be a $m \times n$ matrix with first n columns of Q:

$$Q_n = [q_1, q_2, \dots, q_n]$$
$$Q_{n+1} = [q_1, q_2, \dots, q_n, q_{n+1}]$$

and consider first n columns of $AQ_n = Q_{n+1}\widetilde{H_n}$. The nth column is

$$Aq_n = h_{1n}q_1 + \cdots + h_{nn}q_n + h_{n+1}q_{n+1}$$

which can be used to find q_{n+1}. This recursive computation of columns of unitary matrix Q is Arnoldi iteration (Fasshauer).

2.7 Generalized Minimal Residual Method (GMRES)

The GMRES is an iterative method that solves general non-symmetric linear systems (Walker & Zhou, 1994). The idea is to solve a least squares problem at each step of the iteration (Fasshauer). The GMRES algorithm can be summarized into the following steps:

i. Use Arnoldi method to find q_n.
ii. Find y_n such that the residual $\|r_n\|$ is minimized.
iii. Find x_n by using $x_n = Q_n y_n$.
iv. Repeat till residual vector is minimized sufficiently.

The rate at which the GMRES method converges depends on how the eigenvalues of A are distributed in the plane. If the eigenvalues are clustered away from the origin, the method will converge quickly.

5. Choosing the "Best" Method

Since there are a number of methods available, it is difficult to pinpoint as to which is the "best method" to solve a linear sparse system. Depending on the type of given system and what solution is wanted, a method that is better than the others can be selected for that particular system.

If A is not very large, say, a 1000×1000 matrix, it is easier to choose direct methods. For a symmetric and positive definite matrix, the Cholesky Factorization is a good choice. Direct methods give a very good accuracy and fails rarely. However, such direct methods require the entire factorization to be completed for the results to be useful. It is time consuming and expensive. Additionally sparse matrices may not necessarily decompose into sparse matrices. This causes storage problems and the methods can slow down.

Iterative methods, on the other hand can give a partial result after a small number of iterations. It requires less effort than direction methods and are often easy to program. If accuracy is not important, iterative methods such as CG or GMRES are better for sparse matrices.

The Sherman-Morrison formula requires only $O(n^2)$ operations but it is applicable for rake-one changes only. Moreover, with repeated iterations, the formula destabilizes.

The CG method needs n iterations to obtain an error free convergence but a pretty good approximation can be achieved with a few iterations. It requires only a few matrix-vector multiplications and some dot products per iteration which makes it a computationally inexpensive and numerically stable option. The method only fails if the matrix is not symmetric and positive definite.

GMRES is designed to work with non-symmetric systems (Coban & Lionheart, 2014). For a well-conditioned coefficient matrix, GMRES works a direct solver and an exact solution can be obtained in n steps. The disadvantage is that a large memory is required for storage.

6. CONCLUSION

Linear systems usually contain large sparse matrices which can be difficult when attempting to solve directly. An iterative approach can be taken such as detailed above. Depending on the type of linear system given and the requirements needed such as accuracy, storage, computation time can be conditions in picking a method that best suits the linear system.

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