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SOLUTION OF PARTIAL EIGENVALUE PROBLEM IN LATTICE GAUGE THEORY

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Abstract

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Recently the problem of finding few eigenvalues and the corresponding eigenvectors of large sparse real symmetric matrices arose in some studies of the lattice regularization of the nonabelian gauge theories. We present the program designed to solve this problem. The basis of the algorithm used in the program is the subspace iteration method together with the Rayleigh-Ritz procedure and Chebyshev acceleration. The code is compact and well suited to handle large scale matrices. It is comparable in power with the specialized package ARPACK but is of higher mobility. The code has been checked in computations for matrices of the size up to $O(10^5)$.

Аннотация

Аникеева В.А., Борняков В.Г. Решение частичной проблемы собственных значений в решеточной калибровочной теории: Препринт ИФВЭ 2000-44. – Протвино, 2000. – 4 с., 1 табл., библиогр.: 4.

В последнее время задача нахождения нескольких собственных значений и соответствующих им собственных векторов для разреженных действительных симметричных матриц большого размера стала актуальной в некоторых задачах решеточной регуляризации неабелевых калибровочных теорий. В работе представлена программа для решения этой проблемы. Основой алгоритма, используемого в программе, является метод итерирования подпространства совместно с процедурой Рэлея-Ритца и чебышевским ускорением. Программа компактна и удобна для работы с матрицами большого размера. По эффективности она сравнима со специализированным пакетом ARPACK, но более мобильна. Программа была протестирована на матрицах размера вплоть до $O(10^5)$.

Introduction

The problem under consideration arises in the scope of the lattice field theory. In the lattice regularization of the gauge field theories the gauge fixing is used to study gauge noninvariant observables, e.g. gluon or quark propagators, and also to separate the degrees of freedom, playing the main role in the nonperturbative phenomena.

The gauge fixing conditions of interest are given by the differential equation. Its solutions can be found as extrema of the corresponding gauge fixing functional. For example, for the Landau gauge condition the differential equation and the gauge fixing functional have the following form:

$$\partial_\mu A_\mu(x) = 0, \tag{1}$$

$$F[A^g] = \int d^4x [A^g_\mu(x)]^2, \tag{2}$$

where $A_\mu(x)$ is a gauge potential, $A^g_\mu(x)$ is a gauge potential after the gauge transformation $g(x)$.

Many years ago V.N. Gribov discovered the problem of existence of multiple solutions of this equation. This is called the Gribov problem. In the scope of the nonperturbative gauge fixing this problem can be solved by choosing the global minimum of the functional F. In practice this problem cannot be solved exactly while even an approximate solution requires large resources.

Recently another class of gauge conditions has been suggested [1] to replace the one above. In this case the problem of finding a minimum is replaced by the problem of finding the algebraically smallest eigenvalue and the corresponding eigenfunction of the covariant Laplacian

$$\Delta(A) = D^{ab}_\mu(A) D^{ab}_\mu(A), \qquad D^{ab}_\mu(A) = \delta_{ab}\partial_\mu + i f_{abc} A^c_\mu, \tag{3}$$

$$\Delta(A)\phi(x) = \lambda\phi(x), \tag{4}$$

where f_{abc} are the structure constants of the gauge group. This gauge is called the Laplacian gauge. After the space-time has been discretized in the scope of the lattice regularization, this problem is reduced to the common eigenvalue problem

$$Mv = \lambda v \tag{5}$$

for $N \times N$ real symmetric matrix M of large dimension (up to 10^7).

For the Laplacian center gauge used in the confinement phenomena studies [2] it is necessary to find two eigenvectors with smallest eigenvalues.

1. Description of the program

Our program SIMET designed to solve this problem is based on the algorithm by Rutishauser ([3]) and is written in Fortran77. Attractive features of the program are its compactness, simplicity and some elegance combined with sufficient power. These features provide mobility of the program and easy use on any computer platform.

Program SIMET finds the eigenvalues with maximal absolute values and the corresponding eigenvectors of the real symmetric matrix by the subspace iteration method, which is direct generalization of the power method. One has no need of storing the matrix explicitly. A user should provide the routine to calculate the product of the matrix and arbitrary vector. In this way an essential saving of memory is achieved and the user can deal with matrices of large dimension.

The convergence of the algorithm in the process of finding m eigenvalues with maximal absolute values is linear. It depends on the ratio of the minimal out of the found eigenvalues to the maximal out of the left ones. It is evident that the relative effectiveness of the algorithm depends on the distribution of the eigenvalues and the choice of the internal parameters of the program. More precisely, simultaneous iterations with p ($p > m$) vectors are performed to calculate m eigenvalues with maximal absolute values and this number p affects the convergence rate. Let us enumerate the eigenvalues according to their absolute value: $|\lambda_1| > |\lambda_2| > ... > |\lambda_N|$. Then, the convergence rate of the iterative process is limited by the values of $|\lambda_p/\lambda_m|$ and $\exp(-\cosh^{-1}(|\lambda_m/\lambda_p|))$. The convergence rate is close to the first number when the ratio $|\lambda_1/\lambda_m|$ is large and it is close to the second one when this ratio is of order 1. This algorithm turns out to be rather effective in many practical situations.

The iterative procedure consists of four steps.

1. External loop which includes eigenvalues calculation by the Jacoby method. This step is rather time consuming in comparison with others due to the operations with columns of matrix $X(N, p)$ containing approximations of eigenvectors being searched for. In some sense this is the price for memory saving. The following loop is introduced to reduce the time of calculations by decreasing the number of calls in the external loop.
2. Loop for intermediate calculations including the Chebyshev acceleration.
3. Randomization is used to avoid instabilities of iteration process when the choice of initial subspace is unsuccessful, i.e. p-th column of matrix $X(N, p)$ is replaced by a random vector, being orthogonal to the rest vectors of the basis. This is the simplest way to minimize the probability to lose any of the eigenvectors being searched for. Randomization is performed only during three first calls of loop 1.
4. Check of the solution precision. The calculation of the eigenvalue is finished when relative increase of the corresponding Rayleigh-Ritz ratio turns out to be less than $\varepsilon/10$, where ε is the parameter defined by the user. The convergence of eigenvectors is slower and their errors are calculated more accurately. It is important that for close or equal in absolute value eigenvalues of initial matrix the check of eigenvectors precision is performed simultaneously.

2. Comparison with ARPACK

We made comparison of our program SIMET with the public domain package ARPACK [4]. ARPACK has been used by other authors [2] to solve the eigenvalue problem we consider here.

Our computations were made with a set of matrices of different size with the largest matrix of dimension $N = 196608$ (that corresponds to the lattice with extension $L = 16$ and the gauge group $SU(2)$). Since SIMET finds the eigenvalues maximal in their absolute values, while we need eigenvalues algebraically smallest, we carried out a proper shift of the matrix to make the needed eigenvalues maximal in the absolute values. The discrepancy of the eigenvalues defined as

$$d_n = \frac{|\lambda_{n,AR} - \lambda_{n,SI}|}{|\lambda_{n,AR}|} \tag{6}$$

turned out to be $O(10^{-9})$. The discrepancy for the eigenvectors components, defined in a similar way, was $O(10^{-6})$ (eigenvectors were normalized to 1). This result is quite satisfactory for the problem under consideration. The calculated numbers for the eigenvalues and several components of the first two eigenvectors are given in Table below. The computations were made with a double precision at AlphaServer 8200 in IHEP, Protvino. We found that SIMET is by a factor of 1.5–1.7 slower than ARPACK. This is not quite a noticeable disadvantage of SIMET in view of its simplicity (SIMET code consists of O(500) lines).

Table. Comparison of SIMET and ARPACK. SIMET parameters: $\varepsilon = 1.00\text{E-}10$, $N = 196608$, $m = 2$, $p = 20$.

Eigenvalues

SIMET	ARPACK
1.74962844353513	1.74962844522513
1.75187775426450	1.75187775252235
1.75357796019262	1.75357796006998
1.76045982303397	1.76045981931244

Eigenvectors

SIMET		ARPACK	
#1	#2	#1	#2
1.2121719E-03	-1.1582481E-03	1.2121729E-03	-1.1582472E-03
-4.4862248E-04	-5.7145053E-04	-4.4862305E-04	-5.7145057E-04
-2.0270178E-04	3.1757135E-05	-2.0270198E-04	3.1757151E-05
-1.3595531E-03	7.3657876E-04	-1.3595540E-03	7.3657767E-04
3.0775913E-04	8.5726348E-04	3.0775939E-04	8.5726334E-04
-6.8840846E-04	3.7147894E-04	-6.8840963E-04	3.7147839E-04
-6.7704302E-04	8.6564027E-04	-6.7704293E-04	8.6563912E-04
-2.1420253E-03	6.3581455E-04	-2.1420263E-03	6.3581258E-04
8.1211520E-04	-3.3373447E-05	8.1211587E-04	-3.3372664E-05
-2.1716384E-04	3.1304149E-04	-2.1716431E-04	3.1304157E-04

We, thus, demonstrated that SIMET had high enough speed and precision. The advantage of this program is its simplicity. It can be easily adapted to any dedicated computer used in simulations of the lattice gauge theories. One example of such computer is APE, successfully used by many groups in Italy and Germany and recently installed at JINR, Dubna. This computer is equipped with a high level programming language close in syntax to Fortran. It is easy to adapt SIMET to this computer.

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