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Solving the k-Sparse Eigenvalue Problem with Reinforcement Learning

Li Zhou[1], Lihao Yan[2], Mark A. Caprio[2], Weiguo Gao[1,3] and Chao Yang[4,*]

[1] *School of Mathematical Sciences, Fudan University, Shanghai 200433, P.R. China.*
[2] *Department of Physics, University of Notre Dame, IN 46556, United States.*
[3] *School of Data Science, Fudan University, Shanghai 200433, P.R. China.*
[4] *Computational Research Division, Lawrence Berkeley National Laboratory, CA 94720, United States.*

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Abstract. We examine the possibility of using a reinforcement learning (RL) algorithm to solve large-scale eigenvalue problems in which the desired the eigenvector can be approximated by a sparse vector with at most k nonzero elements, where k is relatively small compare to the dimension of the matrix to be partially diagonalized. This type of problem arises in applications in which the desired eigenvector exhibits localization properties and in large-scale eigenvalue computations in which the amount of computational resource is limited. When the positions of these nonzero elements can be determined, we can obtain the k-sparse approximation to the original problem by computing the eigenvalue of a $k \times k$ submatrix extracted from k rows and columns of the original matrix. We review a previously developed greedy algorithm for incrementally probing the positions of the nonzero elements in a k-sparse approximate eigenvector and show that the greedy algorithm can be improved by using an RL method to refine the selection of k rows and columns of the original matrix. We describe how to represent states, actions, rewards and policies in an RL algorithm designed to solve the k-sparse eigenvalue problem and demonstrate the effectiveness of the RL algorithm on two examples originating from quantum many-body physics.

AMS subject classifications: To be provided by authors

Key words: Large-scale eigenvalue problem, quantum many-body problem, eigenvector localization, reinforcement learning, approximate Q-learning, stochastic sampling, high performance computing.

*Corresponding author. *Email address:* cyang@lbl.gov (C. Yang)

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1 Introduction

Let A be an $n\times n$ sparse symmetric matrix, where n can be very large. We are interested in solving the following problem

$$\min_{\|x\|_0\leq k}\frac{x^TAx}{x^Tx}, \tag{1.1}$$

where $\|\cdot\|_0$ denotes the cardinality of a vector, i.e., the number of non-zero elements of a vector. A vector x that satisfies $\|x\|_0=k$ is called a k-sparse vector. We will refer to (1.1) as a k-sparse eigenvalue problem because the solution to (1.1) is the eigenvector associated with the algebraically smallest eigenvalue of A if the k-sparse constraint $\|x\|_0$ is not imposed. When the k-sparse constrain is imposed, the solution to (1.1) can be obtained from the eigenvector of a submatrix of A with at most k rows and columns.

The k-sparse eigenvalue problem can also be more plainly stated as follows: Select at most k rows and columns of A to form a submatrix A_1 such that the algebraically smallest eigenvalue of A_1 is the smallest among all smallest eigenvalues of all submatrices of dimension at most k. Note that we may replace the minimum in (1.1) by maximum if the eigenvalue of interest is the largest among all eigenvalues. This problem is related to the sparse principal component analysis (PCA) problem in which A is a covariant matrix of the form $A=B^TB$, and minimization is replaced with maximization in (1.1) [10,16,17].

If the eigenvector x^* associated with the algebraically smallest eigenvalue of A has at most k nonzero elements, it is the solution of (1.1). The positions of the nonzero elements of the eigenvector specify the rows and columns of A that defines A_1.

If x^* has more than k nonzero elements, it is not entirely clear how one can obtain the solution to (1.1) efficiently or which rows and columns of A should be extracted to form A_1 whose lowest eigenvalue yields the minimum of the objective function in (1.1). As we will show in Section 5, even if we can compute the smallest eigenvalue of A, simply taking k rows and columns of A corresponding to the k largest components (in magnitude) of the corresponding eigenvector does not necessarily yield the optimal solution to (1.1).

The k-sparse eigenvalue problem is of particular interest when we try to solve a large-scale eigenvalue problem with a limited amount of computational resource. One of the motivations originates from solving a quantum many body problem

$$\mathcal{H}\Psi=\Psi E, \tag{1.2}$$

where $\mathcal{H}$ is a many body Hamiltonian and Ψ is an eigenfunction of $\mathcal{H}$ corresponding to the eigenvalue E. The lowest eigenvalue E_0 and its corresponding eigenfunction form the ground state of the many-body Hamiltonian [23,24,31].

One way to solve (1.2) is to expand Ψ in terms of a linear combination of a finite number of many-body basis functions known as Slater determinants in some well-defined Hilbert space (often referred to as a configuration interaction space), and solve a projected linear eigenvalue problem in that subspace. To obtain an accurate approximation to the solution of (1.2), the dimension of the configuration space may be prohibitively