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主　論　文　の　要　旨

論文題目　A numerical algorithm for the k-th eigenvalue problem of large matrices and its applications
（大規模行列のｋ番目の固有値問題に対する数値アルゴリズムとその応用）

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論　文　内　容　の　要　旨

For a given index k, this thesis presents a numerical algorithm for computing the k-th eigenvalue and its associated eigenvector of a Hermitian definite generalized eigenproblem of large sparse matrices, or the k-th eigenvalue problem, and its applications.

Eigenvalue problems are a fundamental problem in numerical linear algebra, and their numerical solution is essential to various areas of computational science and engineering. Of practical interest is often a subset of eigenvalues and eigenvectors, and a variety of algorithms have been proposed for or have been found to be effective for computing a specific type of subsets, such as a small number of eigenvalues closest to a given point and their associated eigenvectors.

The k-th eigenvalue problem has originated from electronic structure calculations of materials, where the eigenvalue and eigenvector of a material-specific index k play a fundamental role in the research of various material properties. The k-th eigenvalue and its associated eigenvector do not fall into a typical subset at which the existing algorithms are aimed, and all or a substantial number of eigenvalues and eigenvectors have been computed to obtain the k-th eigenvalue and eigenvector.

This thesis proposes an efficient algorithm for computing the k-th eigenvalue and eigenvector with validation of their index, based on Sylvester's law of inertia and the bisection algorithm and by utilizing the Lanczos method and a sparse direct linear solver. Closely related to eigenvalue problems are singular value problems, and the k-th singular value and its associated left and right singular vectors of a large sparse matrix are computed based on the proposed algorithm. Contributions of the thesis are discussed from the perspective of Real-World Data Circulation.