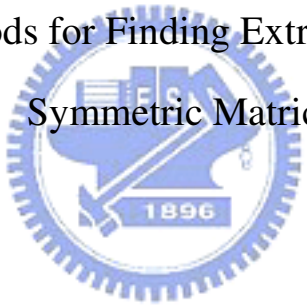
國 立 交 通 大 學

應用數學系

碩 士 論 文

尋找對稱矩陣的極特徵根之疊代方法

Iterative Methods for Finding Extreme Eigenvalues of Symmetric Matrices



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中 華 民 國 九 十 七 年 六 月

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Iterative Methods for Finding Extreme Eigenvalues of Symmetric Matrices

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國 立 交 通 大 學

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摘要

在很多科學的領域，例如物理和化學，有時必須對角化大型的對稱矩陣。最常用來找一些極特徵根的方法是 Davidson 和 Jacobi-Davidson 方法。在這篇論文中，我們同時提出和測試一個命名為『sweep』的方法。在為數不少的帶狀矩陣中，sweep 方法比 Davidson 和 Jacobi-Davidson 方法表現來的好。失去擴充向量的正交化是一個從這些方法延伸出來的重大問題。我們發現解決它的方式是正交化兩次。在未來，我們需要用更多不同形式的矩陣來驗證 sweep 方法的效能。

Iterative Methods for Finding Extreme Eigenvalues of Symmetric Matrices

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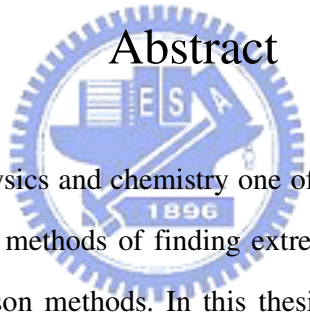

Abstract

In many scientific fields like physics and chemistry one often has to diagonalize large symmetric matrices. The two most popular methods of finding extreme eigenvalues of such large matrices are Davidson and Jacobi-Davidson methods. In this thesis we propose and test a new method, called “sweep method”. We have found that it has better performance than Davidson and Jacobi-Davidson methods for a large class of band matrices. A serious numerical problem obeserved for all these methods is a loss of orthogonality among the expansion vectors. We have found this problem can be avoided by doing two orthogonalizations. In the future, we need more different types of matrices to confirm the efficiency of the sweep method.

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