数学与系统科学研究院

计算数学所学术报告

报告人： **Prof. Houduo Qi**

（ *School of Mathematics, University of Southampton, UK* ）

报告题目：

Newton's method for computing the nearest Euclidean distance matrix

邀请人： 李庆娜 博士

报告时间：2012 年 4 月 18 日（周三）

上午 **10：00-11:30**

报告地点： 科技综合楼三层 **311**

计算数学所报告厅

Abstract：

The Nearest Euclidean distance matrix problem (NEDM) is a fundamental computational problem in applications such as multidimensional scaling and molecular conformation from nuclear magnetic resonance data in computational chemistry. Especially in the latter application, the problem is often a large scale with the number of atoms ranging from a few hundreds to a few thousands.In this paper, we introduce a semismooth Newton method that solves the dual problem of (NEDM). We prove that the method is quadratically convergent.

We then present an application of the Newton method to NEDM with H-weights via an accelerated proximal gradient scheme. We demonstrate the superior performance of the Newton method over existing methods including the latest quadratic semi-definite programming solver.

This research also opens a new avenue towards efficient solution methods for the molecular embedding problem.

欢迎大家参加！