数学与系统科学研究院

计算数学所学术报告

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报告题目：

The Cluster Newton Method and its Improvement for Underdetermined Inverse Problems --- Application to Pharmacokinetics

邀请人：　　白中治 研究员

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报告地点：　　科技综合楼三层 **311**

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Abstract:

An algorithm is proposed for simultaneously finding multiple solutions of an underdetermined inverse problem. The algorithm was developed for an ODE parameter identification problem in pharmacokinetics for which multiple solutions are of interest. The algorithm proceeds by computing a cluster of solutions simultaneously, and is more efficient than algorithms that compute multiple solutions one-by-one because it fits the Jacobian in a collective way using a least squares approach. It is demonstrated numerically that the algorithm finds accurate solutions that are suitably distributed, guided by a priori information on which part of the solution set is of interest, and that it does so much more efficiently than a baseline Levenberg-Marquardt method that computes solutions one-by-one. It is also demonstrated that the algorithm benefits from improved robustness due to an inherent smoothing provided by the least-squares fitting. In the case of pharmacokinetics, underdetermined inverse problems are often given extra constraints to restrain the variety of solutions. We propose a new algorithm based on the two parameters of the Beta distribution for finding a family of solutions which best fit the extra constraints. This allows for a much greater control on the variety of solutions that can be obtained with the CN method. In addition, this algorithm facilitates the task of obtaining pharmacologically feasible parameters.

This work was mainly done by Yasunori Aoki (Uppsala University), Philippe Gaudreau (University of Alberta), and is also joint work with Akihiko Konagaya (Tokyo Institute of Technology), Hans De Sterck (University of Waterloo), and Hassan Safoui (University of Alberta).

欢迎大家参加！