数学与系统科学研究院

计算数学所学术报告

报告人： **Prof. Christine Shoemaker**

（**Cornell University, USA**）

报告题目：

New RBF Algorithms for Nonlinear and Global Optimization and Uncertainty Analysis of Computationally Expensive Simulation Models

邀请人： 戴彧虹研究员

报告时间：**2010** 年 **6** 月 **29** 日（周二）

下午 **4：00**

报告地点： 科技综合楼三层 **311**

计算数学所报告厅

Abstract：

Optimization and uncertainty analyses used in conjunction with complex simulation models are important for using models to make predictions based on observations and for finding optimal designs or policies. Global Optimization and uncertainty analysis typically require a very large number of simulations, often thousands or tens of thousands. However, this approach is not feasible for computationally expensive simulation models that arise in many engineering and science applications.

Our approach to creating more efficient methods for this analysis is to iteratively approximate the objective function or likelihood function f(x) with Radial Basis Functions (RBF). All of our methods are derivative-free.

Our methods differ from most other methods in that we use the results of most previous simulations in the optimization search in each iteration to help build an approximation of the function to be optimized in future optimization iterations. In iteration m, the RBF then approximates $f(x)$ based upon the m values of $f(x_i)$ for x_1, x_2, …,x_m computed in previous iterations of the optimization search.

It is this use of previously evaluated points f (x_i) that is responsible for great savings in computational time. I will review several optimization methods we have developed including a local optimization method ORBIT (that uses trust regions) (Wild et al., 2007) and a global optimization methods, Stochastic RBF (Regis and Shoemaker, 2007, 2009). Stochastic RBF has also been modified to run in parallel. I will give results that compare these algorithms and show significant computational improvements over other methods multiple problems, including complex simulations .

I will also briefly discuss the use of these derivative-based methods in our new uncertainty method SOARS that combines an iterative RBF approximation of the multivariate likelihood function , iterative optimization search, and Markov Chain Monte Carlo. Results show that the computation required by SOARS is less than 1/60 of that required by standard Markov Chain Monte Carlo for accurate uncertainty assessment on two very different engineering applications.

This talk is based primarily on work done jointly with R. Regis and S. Wild in manuscripts and in papers published in INFORMS Jn. of Computing, European Jn. of Operations Research, Jn. of Computational and Graph. Statistics, and SIAM Scientific Computing as well as the Ph.D. theses of Regis and Wild in Operations Research. The SOARS research has been done with Prof. Ruppert and N. Bliznyuk.

Prof. Christine Shoemaker 简介：

CHRISTINE A. SHOEMAKER

EDUCATION

University of California   Mathematics   B.S. 1966

University of Southern California   Mathematics   (advisor: Richard Bellman)   Ph.D. 1971

ACADEMIC POSITIONS

1972-Present   Joseph P. Ripley Professor, Professor, Assoc. Professor, or Asst. Professor, Civil and Environ. Engineering and School of Operations Research and Information Engineering, Cornell University, Ithaca, N.Y.   14853; (607) 255-9233, CAS12@cornell.edu

1985-1988   Chairperson, Department of Environmental Engineering (18 faculty members)

HONORS

Joseph P. Ripley Professorship, Cornell University 2002

Distinguished Member, American Society of Civil Engineers 2006 (highest award given by ASCE)

Fellow, INFORMS (Institute for Operations Research and Management Science-primary US professional organization for Operations Research) 2004

Humboldt Research Prize for senior scientists, from Humboldt Foundation in Germany, 2001.

Fellow, American Geophysical Union, Hydrology Section 2003

Julian Hinds Award, Amer.   Soc. of Civil Engineering (highest award by Water Resources Planning   and Management Division of ASCE) 1999

Fellow, American Society of Civil Engineers (ASCE) 1996

Distinguished Educator Award 1991 from the national Society of Women Engineers (for teaching, research, administration achievements and "as a champion and role model for women in engineering").

SELECTED PUBLICATIONS[1]

Regis, R.G., C.A. Shoemaker, "A Stochastic Radial Basis Function Method for the Global Optimization of Expensive Functions", *INFORMS Jn. of Computing*, 19: 497-509, doi:10.1287/ijoc.1060.0182 2007.

Regis, R.G., C.A. Shoemaker, "Parallel Stochastic Global Optimization Using Radial Basis Functions**," *INFORMS Jn. of Computing*, 21 (3), 411-426, 2009

Regis, R.G. and Shoemaker, C.A. Parallel radial basis function methods for the global optimization of expensive functions. **European Journal of Operational Research** 182(2), 514-535 , 2007

Caffey, H., L-Z Liao, and C.A. Shoemaker, "Parallel Processing of Large Scale, Discrete-Time, Unconstrained Differential Dynamic Programming," **Parallel Computing 19,1003**-1018, 1993.

Eschenbach, E.A., C.A. Shoemaker, and H. Caffey, "Parallel Processing of Stochastic Dynamic Programming for Continuous State Systems with Linear Interpolation" **INFORMS Journal on Computing** 7, pp. 386-401, 1995

Wild, Stefan, Regis, R.G.., Shoemaker, C.A., "ORBIT: Optimization by Radial Basis Function Interpolation in Trust-Regions," SIAM **Journal on Scientific Computing 30**(6) 3197-3219, 2007

Mugunthan, P., C.A. Shoemaker, R. Regis "Comparison of Function Approximation, Heuristic and Derivative-based Methods for Automatic Calibration of Computationally Expensive Groundwater Bioremediation Models," **Water Resources Research (**AGU), 41, W11427, , 2005

Regis, R., C.A.Shoemaker, "Local Function Approximation in Evolutionary Algorithms for the Optimization of Costly Functions**," IEEE Transactions on Evolutionary Computation** 8 (5) 490-505, , 2004

Shoemaker, C.A.., R. Regis: MAPO: using a committee of algorithm-experts for parallel optimization of costly functions. SPAA 2003: 242-243

.Regis, R., and C A.. Shoemaker, "Constrained Global Optimization of Expensive Black Box Functions Using Radial Basis Functions", **Journal of Global Optimization** 31 (1) 153-171, 2005

Tolson B.A., C.A. Shoemaker   Efficient prediction uncertainty approximation in the calibration of environmental simulation models, **Water Resources Research**, 44, W04411, 2008

Montanari A, Shoemaker CA, van de Giesen N, "Introduction to special section on Uncertainty Assessment in Surface and Subsurface Hydrology: An overview of issues and challenges "**Water Resources Research**: 45 W00B00, 2009

SELECTED SYNERGISTIC ACTIVITIES

1. Elected to 15 member Board of Directors for **CUAHSI** (NSF consortium for Hydrology) and appointed to senior Advisory panel for **CLEANER** (NSF consortium for Envir. Engineering).

2. Plenary Speaker Canadian Mathematics Society Conference, Dec. 2009 and for IMA (NSF Center for Mathematics) on Solving Large Scale Parameter Estimation Problems, 2011.

3. Chairman and fund raiser (from UNEP) for **international SCOPE project on groundwater contamination** that had workshops in 6 different countries (including China, Eastern Europe, Latin America, Thailand), 1988-1995.

4. **Teaching and Research:** Prof. Shoemaker works with her Oper. Research/ Applied Math Ph.D. students on new computational optimization algorithms and with her Envir. Engr. Ph.D. students on applying these algorithms to important real environmental problems. Shoemaker developed and currently teaches an interdisciplinary graduate course (co listed in Computer Science, Civil Engr., and Oper. Res. & IE) on heuristic optimization that attracts around 50 graduate students/year from Computer Science and many fields of Engineering.

欢迎大家参加！