Challenges in Computational Mathematics

Friday, September 23, 2005

Convenors: Bob Anderssen and Frank de Hoog,
CSIRO Mathematical and Information Sciences

9:00 – 9:30	**Mike Osborne**, *Australian National University* Multiple shooting revisited
9:30 – 10:00	**Gene Golub**, *Stanford University* Matrices, moments and quadrature with emphasis on least squares problems
10:00 – 10:40	**Georg Bock**,*University of Heidelberg* From parameter estimation to the design of optimal experiments in differential algebraic equations
10:40 – 11:00	*Morning Tea*
11:00 – 11:40	**Åke Björck**, *Linköping University* Recent developments in least squares computations — Bidiagonal decomposition and least squares
11:40 – 12:20	**Gordon Smyth**, *Walter & Eliza Hall Inst. of Med. Res.* Random effects, heteroscedastic regression, algorithms and microarray data analysis
12:20 – 13:30	*Lunch*
13:30 – 14:00	**Richard Brent**, *Australian National University* Challenges in solving large sparse linear systems over finite fields
14:00 – 14:30	**William McLean**, *University of New South Wales* The conditioning of boundary element equations
14:30 – 15:00	**Nick Stokes**, *CSIRO* Material flows — matching micro-scale computations with macroscopic effects
15:00 – 15:30	*Afternoon Tea*
15:30 – 16:00	**Ian Sloan**, *University of New South Wales* The curse of dimensionality
16:00 – 16:30	**Markus Hegland**, *Australian National University* Resolution enhancement of spectra using differentiation

Mike Osborne, *Australian National University*
Multiple Shooting revisited

This talk will consider some stability questions relating to the use of a boundary value problem solver possessing a family relationship with multiple shooting for solving ODE estimation problems when the basic equations possess a strong dichotomy. Questions relating to the provision of compatible boundary conditions will be considered and evidence presented that stiffly stable numerical procedures may be possible.

Gene Golub, *Stanford University*
Matrices, moments and quadrature with emphasis on least squares problems

Given an $n \times n$ symmetric, positive definite matrix A and a real vector u, it is desirable to estimate and bound the quadratic form

$$\frac{u^{\mathrm{T}} F(A) u}{u^{\mathrm{T}} u},$$

where F is a differentiable function. This problem arises in estimating errors of linear systems, computing a parameter in a least squares problem with a quadratic constraint and determining bounds for the perturbations in least squares problems.
We describe a method based on the theory of moments and numerical quadrature for estimating the quadratic form. A basic tool is the Lanczos algorithm which can be used for computing the recursive relationship for orthogonal polynomials.

Georg Bock, *University of Heidelberg*
From parameter estimation to the design of optimal experiments in differential algebraic equations

The quantitative validation of nonlinear differential algebraic and partial differential equations models is a difficult task that requires mathematical methods for parameter estimation, numerical and statistical sensitivity analysis, and the optimal design of experiments. In the talk, we discuss the advantages of the multiple shooting discretization – or rather parametrization – for parameter estimation, and treatment of the discretized BVP as a specially structured, nonlinear equality constraint by Gauss-Newton methods. Based on an assessment of the statistical accuracy of the parameter estimates in terms of confidence regions, efficient optimization methods for the determination of experiments are presented which maximize the information gain subject to feasibility and cost constraints.

Special emphasis is put on questions of robustness: both of the parameter estimation wrt measurement errors – where polyhedral norms are important, and of optimal experiment designs wrt the uncertainty in the parameters. Applications from satellite dynamics, chemical and biochemical reactions will be given. As an outlook, the incorporation of these concepts into real estimation and control schemes are discussed.

Åke Björck, *Linköping University*

Recent developments in least squares computations — Bidiagonal decomposition and least squares

Any rectangular matrix A can be decomposed as $A = UBV^{\mathrm{T}}$, where U and V are orthogonal and B upper (or lower) bidiagonal. In a seminal paper from 1965, Golub and Kahan gave two different, but mathematically equivalent, algorithms for computing this decomposition. The first algorithm uses Householder transformations applied, alternately from left and right, to A. The second algorithm uses two two-term recurrence relations related to a Lanczos process. In this, only matrix-vector products with A and A^{T} are needed.

The Householder algorithm led to the first stable algorithm for computing the SVD of A. This plays a crucial role in direct methods for determining the numerical rank of a matrix A and for solving possibly ill-conditioned, least squares problems. The Lanczos bidiagonalization algorithm forms the core of the Krylov subspace algorithm LSQR. This is the method of choice for solving large sparse least squares problems.

In this talk we review several more recent developments of both algorithms for reduction to bidiagonal form. Paige and Strakoš have shown that reduction to upper bidiagonal form of the matrix $(b\ A)$ provides an elegant way to extract a minimally dimensioned core problem, not only for the linear least squares but also for the (weighted) total least squares problems. For some time it has been known that for a class of least squares problems derived from ill-posed problem the truncated bidiagonal reduction is often superior to the use of truncated SVD. This is related to the popular method of Partial Least Squares (PLS), used in statistics for handling colinearities. In some applications, the familiar loss of orthogonality that occurs in a Lanczos-type bidiagonalization algorithm is not acceptable. This can be cured by applying a (selective) Gram-Schmidt reorthogonalization. We discuss some possible alternatives to this. Several modifications to Householder bidiagonalization have also been suggested in order to improve complexity and accuracy in algorithms for computing the SVD.

Gordon Smyth, *Walter and Eliza Hall Institute of Medical Research*

Random effects, heteroscedastic regression, algorithms and microarray data analysis

Microarrays are one of the technologies underlying the genomic revolution in modern biology. They provide a cheap and accessible way to measure the activity level of genes in an organism, providing measurements for tens of thousands of genes simultaneously. All the usual statistical considerations for designed experiments apply when analysing microarray experiments, but in a massively parallel fashion. Traditional two-colour microarrays especially embody some of the traditional statistical notions of blocking, random effects and non-constant variance. The high throughput nature of the data gives rise to new issues both statistically and computationally. The fact that microarray software is typically used by non-mathematical scientists emphasises the need for reliability and efficiency of the computational algorithms. This talk will describe an approach to microarray data analysis which takes advantage of algorithmic developments for random effects and heteroscedastic regression models. The approach has been implemented in the R computing environment where it takes advantage of the R support for data structures, classes and elementary object-oriented programming.

Richard Brent, *Australian National University*
Challenges in solving large sparse linear systems over finite fields

This talk outlines how very large, sparse linear systems arise in the solution of problems of interest in computational number theory and public-key cryptography, such as the integer factorization and discrete logarithm problems. The linear systems are over finite fields, often the field $GF(2)$ of two elements. We describe some algorithms for solving large sparse linear systems over $GF(2)$, and compare them with algorithms for the real field. In particular, some "iterative" algorithms which are well-known to numerical analysts, such as the conjugate gradient and Lanczos algorithms, can be adapted to work over $GF(2)$, but there are significant differences between algorithms for the real field and for $GF(2)$.

William McLean, *University of New South Wales*
The Conditioning of Boundary Element Equations

We consider Galerkin discretization with standard nodal basis functionsof first-kind boundary integral equations. It is well known that in suchcases the condition number of the stiffness matrix grows as the mesh is refined. We begin by explaining this phenomenon in the familiar case when the mesh is quasi-uniform and then describe some results of joint work with Thanh Tran and Mark Ainsworth on the effect of local refinement. The final part of the talk discusses recent work with Ivan Graham in which the local refinement may be anisotropic, leading to meshes that fail to be shape-regular. This type of refinement arises naturally when one seeks to resolve edge singularities in 3D boundary element methods. We also see how a simple diagonal preconditioning can significantly reduce the condition number.

Nick Stokes, *CSIRO Mathematical and Information Sciences*
Material flows - matching micro-scale computations with macroscopic effects

For complex media in motion which is not governed by a partial differential equation with fixed boundaries, progress can be made by numerically modelling the interactions of smaller parts with more predictable behaviour.

Examples include the various kinds of meshless fluid modelling, and the modelling of granular flows as individual collisions of rigid bodies. The direct numerical simulation of high Reynolds number flows is another. A challenge is that the micro-scale dictates a necessary resolution, which may be very different to the scale of the phenomenon being modelled. It is, for example, feasible to model a mill full of rocks, but not one full of sand, and yet this may represent the progress of the milling process. What is badly needed is a kind of intermediate scale, in which the micro-scale modelling determines a larger scale quasi-continuum behaviour, at which scale further modelling can be performed. This talk will unfortunately not fulfil this need, but will give some indications of the advances that are being made at the micro level.

Ian Sloan, *University of New South Wales*
The curse of dimensionality

Richard Bellman coined the phrase "the curse of dimensionality" to describe the extraordinarily rapid increase in the difficulty of most problems as the number of variables increases. A typical problem is numerical multiple integration, where the cost of any integration formula of product type obviously rises exponentially with the number of variables. Nevertheless, problems with hundreds or even thousands of variables do arise, and are now being tackled successfully. In this talk I will describe recent strategies, mathematical settings and constructions with which suitable integration problems (from mathematical finance, for example) are being successfully handled.

Markus Hegland, *Australian National University*
Resolution enhancement of spectra using differentiation

The analysis of measured spectra, when it reduces to finding the positions and heights of spectral lines, becomes an extremely difficult problem when the lines are closely spaced and broadened to the point where overlapping occurs, and explicit models for the shape of the peaks are unknown. In this talk, I will cover some recent results we obtained by applying a Hilbert space framework to analyse several methods and I will present new enhancement techniques based on numerical differentiation.
This is joint work with Bob Anderssen, of CSIRO Mathematical and Information Sciences.

Reference:

Resolution enhancement of spectra using differentiation, Hegland, Markus; Anderssen, Robert S. Inverse Problems, June 2005, vol. 21, no. 3, pp. 915 – 934(20), `http://www.ingentaconnect.com/content/iop/ip`