Multi-level Monte Carlo in Systems Biology

SATURDAY, MAY 25, 2013
Eckhart 133, 5734 S. University Avenue

ABSTRACT

Multi-level Monte Carlo is a relatively new method that computes expectations of stochastic processes to a desired tolerance significantly faster than previous methods. I will detail the basic idea of multi-level Monte Carlo and show how to implement it in the continuous time Markov chain setting, which is a modeling choice commonly used in the biosciences.
ABSTRACT

The Quadratic Eigenvalue Problem is to find the eigenvalues and eigenvectors of a quadratic matrix pencil of the form: $P(\lambda) = M\lambda^2 + C\lambda + K$, where the matrices $M$, $C$, and $K$ are square matrices. Unfortunately, the problem has not been widely studied because of the intrinsic difficulties with solving the problem in a numerically effective way. Indeed, the state-of-the-art computational techniques are capable of computing only a few extremal eigenvalues and eigenvectors, especially if the matrices are large and sparse, which is often the case in practical applications. On the other hand, the Inverse Quadratic Eigenvalue Problem refers to constructing the matrices $M$, $C$, and $K$, given the complete or partial spectrum and the associated eigenvectors. The inverse quadratic eigenvalue problem is equally important and arises in a wide variety of engineering applications, including mechanical vibrations, aerospace engineering, design of space structures, structural dynamics, etc. Of special practical importance is to construct these matrices from the knowledge of only partial spectrum and the associated eigenvectors, which is computationally challenging. Furthermore, computational techniques must be able to take advantage of the exploitable physical properties, such as the symmetry, positive definiteness, sparsity, etc., which are computational assets for solutions of large and sparse problems.

This talk will deal with two special partial quadratic inverse eigenvalue problems that arise in mechanical vibration and structural dynamics. The first one, Quadratic Partial Eigenvalue Assignment Problem (QPEVAP), arises in controlling dangerous vibrations in mechanical structures. Mathematically, the problem is to find two control feedback matrices such that a small number of eigenvalues of the associated quadratic matrix pencil, which are responsible for dangerous vibrations, are reassigned to suitably chosen ones while keeping the remaining large number of eigenvalues and eigenvectors unchanged. Additionally, for robust and economic control design, these feedback matrices must be constructed in such a way that they have the norms as small as possible and the condition number of the modified quadratic inverse problem is minimized. These considerations give rise to two nonlinear unconstrained optimization problems. The other one, the Finite Element Model Updating Problem (FEMUP), arising in structural dynamics, refers to updating an analytical finite element model so that a set of measured eigenvalues and eigenvectors from a real-life structure are reproduced and the physical and structural properties of the original model are preserved. A properly updated model can be used in confidence for future designs and constructions. Another major application of FEMUP is the damage detections in structures. Solutions of FEMUP also give rise to several constrained nonlinear constrained optimization problems. I will give an overview of the recent developments on computational methods for these difficult nonlinear optimization problems and discuss directions of future research with some open problems.

The talk is interdisciplinary in nature and will be of interests to mathematicians, computational and applied mathematicians, and control and vibration engineers and optimization experts.
Radial basis function (RBF) interpolation – or more generally interpolation with reproducing kernels – uses a positive definite kernel $K$ to reconstruct an unknown function $f$ from its samples $y_i = f(x_i), i = 1, \ldots, N$, obtained at the locations $x_i$ in $\mathbb{R}^d$. In doing so, $f$ is approximated by an expansion of the form $s(x) = \sum_{j=1}^{N} c_j K(x, x_j)$, where the coefficients $\mathbf{c} = (c_1, \ldots, c_N)^T$ are obtained via solution of the interpolation system $K \mathbf{c} = \mathbf{y}$. Here $K = (K(x_i, x_j))_{i,j=1}^{N}$ is often very ill-conditioned and $\mathbf{y} = (y_1, \ldots, y_N)^T$.

In this talk we will introduce a matrix factorization of the form $K = \Psi \Lambda \Phi^T$ of the standard RBF interpolation matrix $K$ in terms of matrices generated by the orthogonal eigenfunctions of the Hilbert-Schmidt integral operator associated with the kernel $K$. This Hilbert-Schmidt SVD is not a traditional singular value decomposition of $K$, but shares some properties with the SVD. Most importantly, the matrix factors are obtained without ever having to form the ill-conditioned matrix $K$.

We will show how the Hilbert-Schmidt SVD leads to a stable algorithm for computation with positive definite kernels and present a particularly simple implementation of the resulting RBF-QR method for a family of so-called compact Matérn kernels. We will illustrate our algorithm with a standard interpolation example, and with an application to the determination of “optimal” RBF shape parameters via cross-validation.

This is joint work with Mike McCourt.
Automatic algorithms are designed to provide the desired answer to within a user-specified error tolerance. The number of function values required is not specified by the user but determined adaptively by the algorithm. Commonly used automatic numerical integration algorithms may fail to give the correct answer, either because the integrand is too spiky or because the error estimation method is faulty. We present new algorithms for approximating univariate and multivariate integrals that estimate the error differently than before. By considering cones of integrands, we can provide theoretical guarantees that these algorithms do provide the correct answer. We are also able to show that their computational cost is optimal. These new algorithms, and those under development, will become part of the Guaranteed Automatic Integration Library (GAIL), which will be briefly described. This is joint work with Sou-Cheng Choi, Yuhan Ding, Lan Jiang, and Yizhi Zhang.
We present a treecode-accelerated boundary integral (TABI) solver for electrostatics of solvated proteins described by the linear Poisson-Boltzmann equation. The method employs a well-conditioned boundary integral formulation for the electrostatic potential and its normal derivative on the molecular surface. The protein surface is triangulated by MSMS and the integral equations are discretized by centroid collocation. The linear system is solved by GMRES iteration and the matrix-vector product is carried out by a Cartesian treecode which reduces the cost from $O(N^2)$ to $O(N \log N)$, where $N$ is the number of faces in the triangulation. We compare TABI results with those obtained using the grid-based APBS code, and we also present parallel TABI simulations using up to eight processors. The TABI solver exhibits good serial and parallel performance combined with relatively simple implementation, efficient memory usage, and geometric adaptability. This is joint work with Weihua Geng (University of Alabama, Tuscaloosa).
We introduce a new framework for the multiphysical modeling and multiscale computation of nano-optical responses. The semi-classical theory treats the evolution of the electromagnetic field and the motion of the charged particles self-consistently by coupling Maxwell equations with Quantum Mechanics. To overcome the numerical challenge of solving high dimensional many body Schrodinger equations involved, we adopt the Time Dependent Current Density Functional Theory (TD-CDFT). In the regime of linear responses, this leads to a linear system of equations determining the electromagnetic field as well as the current and electron densities simultaneously. A self-consistent multiscale method is proposed to deal with the well separated space scales. Numerical examples are presented to illustrate the resonant condition.
ABSTRACT

Many materials problems require the accuracy of atomistic modeling in small regions, such as the neighborhood of a crack tip. However, these localized defects typically interact through long-range elastic fields with a much larger region that cannot be computed atomistically. Materials scientists have proposed many methods to compute solutions to these multiscale problems by coupling atomistic models near a localized defect with continuum models where the deformation is nearly uniform on the atomistic scale.

During the past several years, a theoretical structure has been given to the description and formulation of atomistic-to-continuum coupling methods, and corresponding numerical analysis and benchmark computational experiments have clarified the relation between the various methods and their sources of error. Our theoretical foundation has enabled the development of more accurate and efficient coupling methods.
Gossip Algorithm for Principal Component Analysis

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ABSTRACT

Eigenvectors of data matrices play an important role in many computational problems, ranging from signal processing to machine learning and control. For instance, most algorithms for positioning a collection of wireless devices on the basis of pairwise distance measurements require the computation of eigenvectors of the distances matrix. While eigenvector calculation is a standard topic in numerical linear algebra, it becomes challenging under severe communication or computation constraints, or in absence of central scheduling. In this work, we investigate the problem of computing the leading eigenvectors of a large data matrix through gossip algorithms. The proposed algorithm amounts to iteratively apply independent random sparsification of the original matrix and average the resulting normalized vectors. This can be viewed as a generalization of gossip algorithms for consensus, but the resulting dynamics is significantly more intricate. Our analysis is based on controlling the convergence to stationarity of the associated Furstenberg Markov chain.
Problems, such as finding optimal reaction paths, require minimizing an integral involving an exponential of a function. Conventional minimization methods are not well suited to such problems because they assume the ability to evaluate the objective function, but there seem to be no reasonable higher order approximations for integrals of this type. If the problem is expressed as a dynamical system performing gradient descent, it is possible to do scaling to remove exponential factors. This permits the use of higher order approximations as well as solution methods based on a local linear model. For the case of computing a curve rather than a function, there is another difficulty, namely, arbitrariness in its parameterization. This requires the imposition of a constraint, which in the continuum problem is orthogonal to the direct of descent. Such orthogonality guarantees unconditional descent. Fortunately, it is possible to maintain orthogonality for a discretized problem. This is joint work with R. Zhao, H. Huang, M. Wolff, and C. Post. (Another off-label use for ODE methods is randomization, which could be the subject of another talk.)
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The Gaussian Wave Packet Transform: Efficient Computation of the Semi-classical Limit of the Schroedinger Equation

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ABSTRACT

An efficient method for simulating the propagation of a localized solution of the Schroedinger equation near the semiclassical limit is presented. The method is based on a time dependent transformation closely related to Gaussian wave packets and yields a Schroedinger type equation that is very amenable to numerical solution in the semi-classical limit. The wavefunction can be reconstructed from the transformed wavefunction whereas expectation values can easily be evaluated directly from the transformed wavefunction. The number of grid points needed per degree of freedom is small enough that computations in dimensions of up to 4 or 5 are feasible without the use of any basis thinning procedures. This is joint work with Giovanni Russo.