"Numerical Marginalization with Applications to Physics and to the Sampling of Stochastic Differential Equations"

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Summary

The fast multiscale sampling tools we had developed in previous years have been applied to the sampling of the solutions of stochastic differential equations, as well as to problems in material science.

In previous years the mathematics department at LBNL developed multiscale sampling techniques based on new fast methods for computing marginals. These marginalization techniques use a representation of renormalized Hamiltonians in terms of conditional expectations, which can then be evaluated on the computer with the help of rapidly convergent series.

One application of these ideas is to the sampling of solutions of stochastic differential equations conditioned by initial or final data, something one has to do e.g. in filtering (the estimation of the state of a system on the basis of an uncertain model and noisy partial data). For linear systems the filtering problem is solved by the Kalman filter; for nonlinear problem there is currently no good general solution. In principle particle filters should solve the problem but they are typically too costly of computer time to be very useful.

Estimation via a particle filter can be reduced to the sampling of a Hamiltonian density to which our tools apply. One way to use marginals in this problem is via parallel marginalization- the parallel updating of samples of the original problem and of a sequence of its marginals, accompanied by swaps of information between levels subject to a consistency requirement. This is an effective technique because marginals of a given density equilibrate faster than the initial density. The applications so far include test problems as well as the prediction of the meanders of the Kuroshio current off Japan from shore measurements.

Another, very different, application, is to the sampling of the Anderson-Edwards spin glass model in three dimensions, an important model in material science. Here it turned out that sampling techniques based on Markov chains fail, because the chains get trapped in the numerous local free energy minima. We therefore devised a chainless algorithm as follows: We divided the lattice on which the spins live into a nested sequence of sublattices; if the marginals are known, and if the complement of each sublattice with respect to the next smaller lattice consists of

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relatively independent spins, then one can obtain a sample independent of any previous sample via a top-down sweep, in which a sequence of growing lattices is sampled given a seed sample for the smallest sublattice.

The problem is to find the marginals. This is done by the renormalization technique mentioned above, with the samples needed for estimating the marginals bootstrapped as part of the global sampling. The most difficult part of this algorithm turned out to be the factoring of the three-dimensional lattice so that the relative independence condition be satisfied for each sublattice.

We have now a working program and have checked that the results are consistent with what is known is special cases. We are just beginning to confront issues where previous knowledge is wanting.

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