Learning Monte Carlo

By Francis Sullivan

James Gubernatis, Naoki Kawashima, and Philipp Werner have produced a detailed and comprehensive treatment of computational algorithms and techniques for quantum Monte Carlo in their book, *Quantum Monte Carlo Methods*. Each important algorithm is presented as a way of treating some aspect of a significant class of problems in computational modeling. First, the authors give the necessary physical and mathematical background; they then describe the algorithm and summarize it as clearly stated pseudocode. The presentation via pseudocode is an especially appealing feature: starting from the pseudocode, one could easily construct a working program in, say, Matlab, which could then be refined into a high-performance “real” code in C, Fortran, or another compiled language of choice.

The book is divided into four major parts plus “Other Topics” and several appendices dealing with important but technical mathematical and algorithmic details. The authors start gently in Part I, first explaining the basics of probability and random sampling, Markov chains, and their convergence criteria. Next, they cover the notions of detailed balance, heat-bath algorithms, and the classical Ising model. A section on data analysis follows before the basic cluster and “worm” algorithms are introduced.

The end of Part I is Chapter 5, and it stands as a self-contained primer on quantum Monte Carlo. Here, we find the initial discussion of the difference between classical Monte Carlo, where the partition function is a sum over classical states, and quantum Monte Carlo, where the partition function is the trace of the self-adjoint operator (¼ Hermitian) exp(–βH), for inverse temperature β and Hamiltonian H, which

is itself a Hermitian operator. It's very important that readers understand how this turns a $d$-dimensional quantum problem into a $d + 1$ dimensional classical problem, so the authors proceed with great care. Moreover, understanding that the matrix exponential $\exp(-\beta H)$ is a self-adjoint operator when $H$ itself is self-adjoint requires some understanding of the spectral theory of operators. I was a little surprised that the authors assume readers will have this background and not know basic probability theory, but I think it’s safe to bet that the authors know their audience better than I do.

The authors remark that some techniques are introduced in Chapter 5 to present key ideas to prepare for the heavy lifting in Parts II (“Finite Temperature”) and III (“Zero Temperature”). They cover the two main topics of quantum Monte Carlo clearly, carefully, and thoroughly. The foundation that was laid in Part I does an excellent job of supporting the details in Parts II and III.

But as a mathematician and algorithm designer, I have some quibbles. Virtually all Markov chain Monte Carlo (MCMC) algorithms in use today are known to converge to the limit distribution only after an exponential number of steps. This means that to be completely rigorous, one would have to equilibrate a very long time and wait—for perhaps years—between samples. So how is it that reasonable-length computing times give useful physical results? The answer is that practitioners use their physical intuition when examining numerical and graphical results to determine if they look reasonable. In the present case, this is explained quite clearly in the section on equilibration. But, as it happens, there are polynomial time MCMC algorithms for a few problems, including the classical Ising model. I think it would have been helpful for the authors to at least mention this rather large body of research.

Part IV (“Other Topics”) consists of two chapters, the first covering more advanced topics in probability and statistics relevant to quantum Monte Carlo and the second dealing with the important subject of parallelization. As the authors say, big computers come into their own on big problems of which quantum Monte Carlo is certainly one. The central question is, as usual, how to parallelize, especially in the case of loop or cluster algorithms. In this connection, the authors discuss how to parallelize

the famous union-find algorithm that’s central to keeping track of evolving clusters. My only complaint here concerns the authors’ treatment of the union-find algorithm, an extremely important component of loop-cluster methods. This algorithm is famous because its complexity per operation is governed by the inverse Ackerman function, that is, faster than iterated logs and barely above $O(1)$. This remarkable result and its proof are both due to Turing award winner Robert Tarjan and was published in 1975, although the basic idea seems to have been discovered slightly later by the physics community, only without the complexity proof. The presentation of union-find given in the book under review includes a careful explanation of Tarjan’s path compression idea, so I think his work should have been cited.

Ultimately, I find this to be a valuable and well-constructed manual on quantum Monte Carlo. Anyone who works through this book will be equipped to develop software and carry out any of the most extensively used quantum Monte Carlo simulations using methods that are the best understood and most popular today. The authors are clearly experienced experts.

Francis Sullivan is a mathematician and computational scientist with just enough background in physics to induce feelings of wonder, awe, confusion, and skepticism in himself and those nearby. In his role as director of the IDA Center for Computing Sciences he focuses on applications of leading-edge computational science to problems of interest to the US Department of Defense. Sullivan is a former editor in chief of CiSE and a founder of one of its predecessor publications, IEEE Computational Science and Engineering. Contact him at fran@super.org.