Research statement

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I have been doubly surprised by my career trajectory through graduate school: my mathematical exposure up to that point had been solely deterministic. Namely, I am pursuing interests in applications of probability, with extensive use of statistical methods.

Over the last few years, I have become fascinated with the ways we can make quantitative statements about random events. The keys, of course, are laws of large numbers and central limit theorems. Probability is endlessly fascinating: it is amenable to intuitive, elementary exposition; it is of value to the general undergraduate as well as the science/technology major; and problems in probability permit intriguing combinations of experimental and analytical attack.

Statistics goes hand in hand with probability: the latter uses known laws to predict likelihoods of future events; the former uses past events to infer likely laws governing the underlying models which produced the events. Statistics is the single most practical discipline I know, and I can share my appreciation for it with my students.

In this note, I summarize my dissertation as well as near-future research.

Dissertation

My current research centers on Markov chain Monte Carlo methods in statistical mechanics. This includes side work on lattice percolation and self-avoiding walks; my thesis topic is critical behavior for the model of random spatial permutations. This project lies at the crossroads of probability theory, statistical mechanics, functional analysis, statistics, and numerical methods.

The random-spatial-permutation model arises in the study of the Bose gas, although it is also of intrinsic probabilistic interest; its history includes Bose-Einstein, Feynman, Penrose-Onsager, Sütő [Sütő1, Sütő2], and Ueltschi-Betz [BU07, BU08]. Random permutations arise physically when one symmetrizes the N-boson Hamiltonian with pair interactions, then applies a multi-particle Feynman-Kac formula and a cluster expansion.

Definitions. The state space is $\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N$, where $\Lambda = [0, L]^3$ with periodic boundary conditions; point positions are $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$ for $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \Lambda$. (See figure 1.) One of two distinct Hamiltonians may be used. In one, relevant to the Bose gas, we have

$$H_B(\mathbf{X}, \pi) = \frac{T}{4} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{i<j} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)})$$

where $T = 1/\beta$ and the V terms are interactions between permutation jumps. (The temperature scale factor $T/4$, not $\beta/4$, is surprising but correct for the Bose-gas derivation of the Hamiltonian.) In the second form of the Hamiltonian, we instead use interactions which are dependent solely on cycle length:

$$H(\mathbf{X}, \pi) = \frac{T}{4} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{\ell=1}^{N} \alpha_\ell r_\ell(\pi),$$

where $r_\ell(\pi)$ is the number of ℓ-cycles in π and the α_ℓ's are free parameters, called cycle weights. One ultimately hopes to choose the α_ℓ's appropriately for the Bose gas; even if not, the model is well-defined and of its own interest.

One may hold point positions fixed, e.g. on the unit lattice; this approach has been taken for all simulations done up to the present. Alternatively, one may integrate over all positions in Λ; here, several analytical results are available. In either case, the point positions $\mathbf{X}$ cease to be free parameters and one obtains a Gibbs probability distribution for permutations $\pi \in \mathcal{S}_N$: namely, $P(\pi) = e^{-H(\pi)}/Z$ where the normalizing factor Z is the partition function.

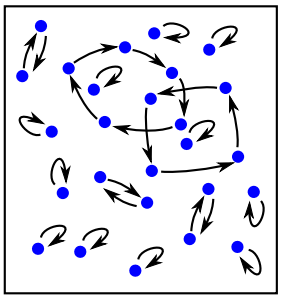

Figure 1: A spatial permutation.

Onset of long cycles. What is a typical permutation in this temperature-dependent probability distribution on $\mathcal{S}_N$? As $T \to \infty$, the probability measure becomes supported only on the identity permutation. For large but finite T, there are tiny islands of 2-cycles, 3-cycles, etc. On the other hand, as $T \to 0$, length-dependent terms go to zero, and the probability measure approaches the uniform distribution on $\mathcal{S}_N$. For intermediate T, the length $\|\pi(\mathbf{x}) - \mathbf{x}\|$ of each permutation jump remains small, increasing smoothly as T drops.

For T above a critical temperature T_c, all cycles are short: two-cycles, three-cycles, and so on. We find $T_c \approx 6.8$, and positive α terms increase T_c. At T_c, though, there is a phase transition: for $T < T_c$ jump lengths remain short but *long cycles form*. Quantitatively, let $\ell_{\max}$ be the length of the longest cycle in π, with $\langle \ell_{\max} \rangle$ its mean over all permutations. We observe that for $T > T_c$, $\langle \ell_{\max} \rangle$ is constant as $N \to \infty$: cycles remain finite. For $T < T_c$, on the other hand, $\langle \ell_{\max} \rangle$ scales with N: there are arbitrarily long cycles, or infinite cycles, in the infinite-volume limit.

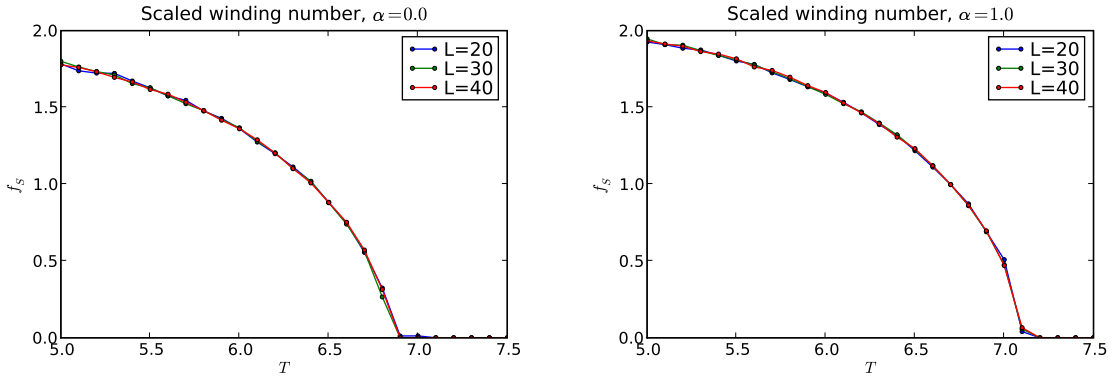

Figure 2: Order parameter f_S for finite systems, with $\alpha = 0.0, 1.0$. Interactions increase the critical temperature.

Various order parameters may be defined; one such is the so-called scaled winding number

shown in figure 2. All of them, including $\langle \ell_{\max} \rangle / N$, exhibit a behavior like that shown in the figure: as L increases, the curve becomes non-analytic at T_c, zero to the right (no long cycles), and non-zero to the left (more and more points are in long cycles). For finite L, the curve remains analytic; finite-size effects persist.

Strengths of the model. Feynman's claim is that Bose-Einstein condensation occurs if and only if there are infinite cycles in the infinite-volume limit. The central point of this approach is that the system energy has been recast in terms of permutations, which are amenable to analysis and simulation. Furthermore, interactions between permutations are recast as collision probabilities between Brownian bridges in Feynman time. These Brownian bridges are in turn integrated out, resulting in a model which lends itself readily to simulations without the need for CPU-intensive path-integral Monte Carlo (PIMC). This permits a new perspective on the venerable question: how does the critical temperature of Bose-Einstein condensation depend on inter-particle interaction strength?

Obtaining a full answer to this question is a long-term project. Breaking it into manageable pieces, my advisor Daniel Ueltschi and I first consider the cycle-weight Hamiltonian with point positions on the unit lattice. Through careful use of MCMC algorithms, statistical analysis, and finite-size scaling, we are able to quantify the dependence of critical temperature on interaction strength for certain cases.

Future plans

The model of random spatial permutations has great interest for me: I will focus much of my attention on it over the next few years, as I also diversify my interests.

Our current MCMC algorithm has execution time which is $O(N^2)$, albeit with a small constant of proportionality. Simulations with $N = 216,000$ points are currently tractable; with a truly $O(N)$ algorithm we will be able to handle larger system sizes, which will in turn reduce our dependence on finite-size scaling methods. Ongoing collaboration led by Daniel Gandolfo of the University of Marseille addresses this issue.

The current algorithm admits only even winding numbers. We believe this to be a non-fatal drawback. For my dissertation work I have developed a worm algorithm which admits winding numbers of both parities. It has an elegant structure, and I have proved much about it. Its only drawback its long stopping time. I hope to resolve this issue in consultation with path-integral Monte Carlo (PIMC) practitioners.

Use of the physical Hamiltonian in place of the cycle-weight Hamiltonian will bring my simulations closer to those of the Bose gas. The physical Hamiltonian is more CPU-intensive to simulate; clever non-stochastic approximation of the necessary Brownian-bridge integral may help.

The other key component to simulating the true Bose gas is the use of continuum (off-lattice) point positions. This eminently doable, although not within my dissertation time-frame; it is a primary goal for my first post-graduate year.

The work of Ueltschi and Betz provides analytical results only for small cycle weights; my current simulations do not have this requirement. Guided by experimental results, we

may be able to either prove that the small-cycle-weight hypothesis is not necessary, or to formulate and prove conjectures about the non-small-cycle-weight case.

Recent collaboration with Tom Kennedy's self-avoiding-walk-bridge group holds computational, conjectural, and theoretical opportunities.

Lastly, recent discussions between myself and Tom LaGatta — another Arizona student completing his PhD this year — suggest a fascinating collaborative project involving best matchings (non-uniformly-weighted random bijections) between Poisson point processes.

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