MCMC methods for random spatial permutations

Shift in critical temperature for the cycle-weight model

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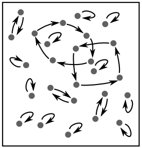
January 13, 2010

The probability model

State space: $\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N$, where $\Lambda = [0,L]^3$ with periodic boundary conditions.
Point positions: $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$ for $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \Lambda$.



Hamiltonian, where $T = 1/\beta$ and $r_\ell(\pi)$ is the number of ℓ-cycles in π:

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

- The first term discourages long permutation jumps, moreso for higher T.
- The temperature scale factor $T/4$, not $\beta/4$, is surprising but correct for the Bose-gas derivation of the Hamiltonian.
- The second term discourages cycles of length ℓ, moreso for higher α_ℓ. These interactions are not between points, but rather between permutation jumps.

The probability model

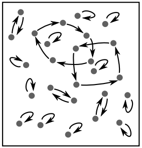
Fixed point positions (quenched model — includes all simulations done up to the present on the cubic unit lattice with $N = L^3$):

$$P_{\mathbf{X}}(\pi) = \frac{1}{Y(\Lambda, \mathbf{X})} e^{-H(\mathbf{X},\pi)}, \quad Y(\Lambda, \mathbf{X}) = \sum_{\sigma \in \mathcal{S}_N} e^{-H(\mathbf{X},\sigma)}.$$

Varying positions (annealed model — many theoretical results are available):

$$P(\pi) = \frac{1}{Z(\Lambda, N)} e^{-H(\mathbf{X},\pi)}, \quad Z(\Lambda, N) = \frac{1}{N!} \int_{\Lambda^N} Y(\Lambda, \mathbf{X})\, d\mathbf{X}.$$

In either case, we write the expectation of an RV $S(\pi)$ as $\mathbb{E}[S] = \sum_{\pi \in \mathcal{S}_N} P(\pi) S(\pi)$.



Feynman (1953) studied long cycles in the context of Bose-Einstein condensation for interacting systems. See also Sütő (1993, 2002), and papers of Betz and Ueltschi.

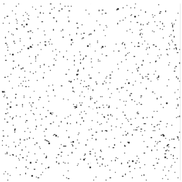
The probability model: intuition

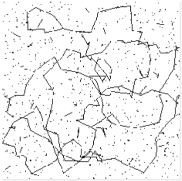
What does a typical random spatial permutation actually look like? (Recall $H(\mathbf{X},\pi) = \frac{T}{4}\sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{\ell=1}^{N} \alpha_\ell r_\ell(\pi)$.)

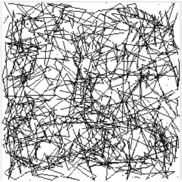
- As $T \to \infty$, the probability measure becomes supported only on the identity permutation. Large but finite T: there are tiny islands of 2-cycles, 3-cycles, etc.
- As $T \to 0$, length-dependent terms go to zero. The probability measure approaches the uniform distribution on $\mathcal{S}_N$: all π's are equally likely.

For intermediate T, things get more interesting:

- The length of each permutation jump, $\|\pi(\mathbf{x}) - \mathbf{x}\|$, remains small.
- Above a critical temperature T_c, all cycles are short: 2-cycles, 3-cycles, etc. $T_c \approx 6.86$, and positive α terms increase T_c.
- Phase transition at T_c: below T_c, jump lengths remain short but *long cycles form*. Order-parameter RVs f_I, f_M, f_W, f_S quantify this; ξ is correlation length.
- Figures: high T, medium but subcritical T, and low T.



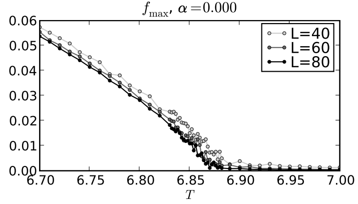


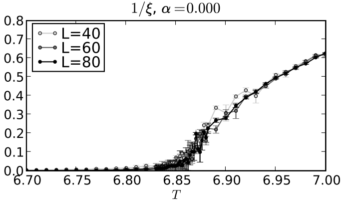


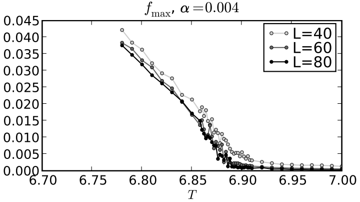
Behavior of order parameters as functions of L, T, and α.

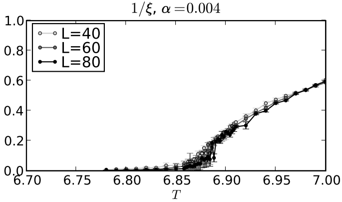
$f_M = \mathbb{E}[\ell_{\max}]/N$ is left-sided; $1/\xi$ is right-sided. All order-parameter plots tend to the right as α increases, i.e. $\Delta T_c(\alpha) = \frac{T_c(\alpha) - T_c(0)}{T_c(0)}$ is positive for small positive α.

Goal: quantify $\Delta T_c(\alpha)$'s first-order dependence on α.









Known results and conjectures

Recall $H(\mathbf{X}, \pi) = \frac{T}{4} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{\ell=1}^{N} \alpha_\ell r_\ell(\pi)$. We have the following models:

- Non-interacting model: $\alpha_\ell \equiv 0$.
- Two-cycle model: $\alpha_2 = \alpha$ and other cycle weights are zero.
- Ewens model: α_ℓ is constant in ℓ.
- General-cycle model: No restrictions on α_ℓ.

Known results for the continuum (obtained largely using Fourier methods):

- $\Delta T_c(\alpha)$ is known (to first order in α) for two-cycle interactions (Betz and Ueltschi, CMP 2008) and small cycle weights (Betz and Ueltschi 2008). (This taps into a long and controversial history in the physics literature: see Baym et al., EJP B 2001, or Seiringer and Ueltschi, PRB 2009, for surveys.) The critical (ρ, T, α) manifold relates ρ_c to T_c.

$$\rho_c(\alpha) \approx \sum_{\ell \geq 1} e^{-\alpha_\ell} \int_{\mathbb{R}^3} e^{-\ell\, 4\pi^2 \beta \|\mathbf{k}\|^2} \, d\mathbf{k} = \frac{1}{(4\pi\beta)^{3/2}} \sum_{\ell \geq 1} e^{-\alpha_\ell} \ell^{-3/2}$$

$$\Delta T_c(\alpha) \approx c\rho^{1/3}\alpha, \quad \text{for } \alpha \approx 0, \text{ with } c = 4\pi\zeta(3/2)^{-2/3} e^{2\alpha/3} \approx 0.66 \text{ when } \rho = 1.$$

Metropolis sampling

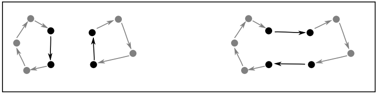
The expectation of a random variable S (e.g. f_W, f_M, f_I, f_S, ξ) is

$$\mathbb{E}[S] = \sum_{\pi \in \mathcal{S}_N} P(\pi) S(\pi).$$

The number of permutations, $N!$, grows intractably in N. The expectation is instead estimated by summing over some number M (10^4 to 10^6) typical permutations. The sample mean is now a random variable with its own variance.

The usual technical issues of Markov chain Monte Carlo (MCMC) methods are known and handled in my simulations and dissertation: thermalization time, proofs of detailed balance, autocorrelation, batched means, and quantification of variance of sample means.

Metropolis step (analogue of single spin-flips for the Ising model): swap permutation arrows which end at nearest-neighbor lattice sites. This either splits a common cycle, or merges disjoint cycles:



As usual, the proposed change is accepted with probability $\min\{1, e^{-\Delta H}\}$.

Computational results: ΔT_c

Raw MCMC data yield $S(L,T,\alpha)$ plots as above, for each order parameter S.
Finite-size scaling (see Pelissetto and Vicari, `arXiv:cond-mat/0012164`, for a survey) determines the critical temperature $T_c(\alpha)$.

Define reduced temperature $t = \frac{T-T_c(\alpha)}{T_c(\alpha)}$, and correlation length ξ as above.

Hypotheses: (1) At infinite volume, $S \sim |-t|^\rho$ and $\xi \sim |t|^{-\nu}$ (power-law behavior).
(2) Finite-volume corrections enter only through a universal function Q_S of the ratio L/ξ:

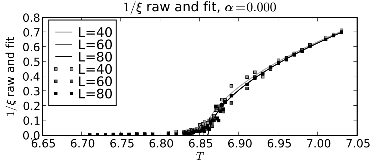
$$S(L,T,\alpha) = L^{-\rho/\nu} Q_S((L/\xi)^{1/\nu}) = L^{-\rho/\nu} Q_S(L^{1/\nu} t)$$

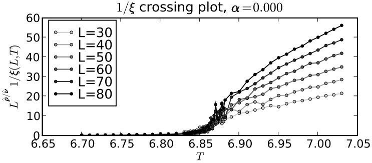
Method:

- Estimate critical exponents ρ, ν via power-law regression on MCMC data plots.
- Plot $L^{\hat{\rho}/\hat{\nu}} S(L,T,\alpha)$ as function of T. Since $t=0$ at $T_c(\alpha)$, these plots for different L cross at $T_c(\alpha)$.
- Having estimated $\hat{\rho}$, $\hat{\nu}$, and $\hat{T}_c(\alpha)$, plot $L^{\hat{\rho}/\hat{\nu}} S(L,T,\alpha)$ as function of $L^{1/\hat{\nu}} \hat{t}$. This causes all curves to collapse, confirming the FSS hypothesis.
- Regress $\Delta \hat{T}_c(\alpha)$ on α to estimate the constant c.

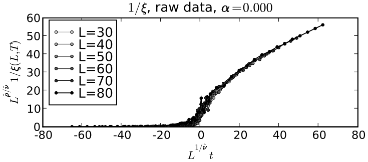
Computational results: ΔT_c

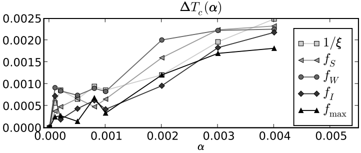
Raw data vs. power-law fit for $1/\xi$ with $\alpha = 0$, followed by crossing plot:





Collapse plot for $1/\xi$ with $\alpha = 0$, followed by $\Delta T_c(\alpha)$ vs. α:





We find $T_c(0) \approx 6.683 \pm 0.003$ and $c \approx 0.665 \pm 0.067$ for Ewens weights on the lattice. For small cycle weights on the continuum, Betz and Ueltschi have $T_c(0) \approx 6.625$ and $c \approx 0.667$. Conclusions: (1) Lattice structure modifies the critical temperature; (2) the α-dependent shift in critical temperature is unaffected.

Other work

Dissertation items not presented today:

- Precise exposition of the theory of autocorrelation estimators for exponentially correlated Markov processes. Precise quantification of the advantages and non-advantages of batched means.
- A worm algorithm permits odd winding numbers and has an elegant theory. However, it has a stopping-time problem.
- Finite-size scaling details.
- Mean length of longest cycle as a fraction of the number of sites in long cycles recovers work of Shepp and Lloyd (1966) for non-spatial uniform permutations.

For the future (postdoctoral):

- Use varying (annealed) point positions on the continuum. This samples from the true point distribution.
- Replace cycle-weight interactions in the Hamiltonian with those derived from the true Bose-gas model. Analytical as well as simulational work is needed in order to make this computationally tractable.

For more information, please visit http://math.arizona.edu/~kerl.

Thank you for attending!