Monte Carlo methods for interacting spatial permutations

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April 2, 2008

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Outline

Acknowledgements

We implement Monte Carlo techniques for the following:

- `arXiv:cond-mat/0703315` (Gandolfo, Ruiz, Ueltschi): describes the non-interacting model. Referred to herein as the GRU paper. (Monte Carlo results were obtained by Gandolfo and Ruiz; we have reproduced their results.)
- `arXiv:0711.1188` (Betz, Ueltschi): Describes the interacting model in detail. The U07 paper (next) summarizes much of the content of this longer paper.
- `arXiv:0712.2443v3` (Ueltschi): Describes the interacting model. Referred to herein as the U07 paper.

This work (spring 2008) is supported by NSF grant DMS-0601075.

Many thanks to the following people for multiple insights: Daniel Ueltschi, Tom Kennedy, Janek Wehr, Ben Dyhr.

Review of spatial random permutations

Review of spatial random permutations

Daniel's talk last week described the Feynman-Kac representation for the Bose gas. The Hamiltonian is

$$\mathbf{H} = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j} U(x_i - x_j) \qquad \text{in } L^2_{\text{sym}}(\Lambda^N)$$

Then $\mathrm{Tr}\, \mathrm{e}{-}\beta\mathbf{H}$ is

$$\sum_{\pi} \frac{1}{N!} \int \mathrm{d}x_1 \ldots \mathrm{d}x_N \int \mathrm{d}W^{2\beta}_{x_1 x_{\pi(1)}}(w_1) \ldots \mathrm{d}W^{2\beta}_{x_N x_{\pi(N)}}(w_N)$$
$$\exp\Big\{-\tfrac{1}{2} \sum_{i<j} \int_0^{2\beta} U\big(w_i(s) - w_j(s)\big) \mathrm{d}s\Big\}$$

Review of spatial random permutations

Write this as

$$\mathrm{Tr}\, \mathrm{e}{-\beta \mathbf{H}} = \frac{1}{N!} \int_{\Lambda^N} \mathrm{d}\mathbf{x} \sum_{\pi} \mathrm{e}{-H(\mathbf{x}, \pi)}$$

where

$$\mathrm{e}{-H(\mathbf{x}, \pi)} = \Big[\prod_{i=1}^{N} \mathrm{d}W^{2\beta}_{x_i x_{\pi(i)}}(\omega_i) \Big] \exp\Big\{ -\tfrac{1}{2} \sum_{i<j} \int_0^{2\beta} U\big(w_i(s) - w_j(s)\big) \mathrm{d}s \Big\}.$$

After cluster expansion,

$$H(\mathbf{x}, \pi) = \frac{1}{4\beta} \sum_{i=1}^{N} |x_i - x_{\pi(i)}|^2 + \sum_{i<j} V(x_i, x_{\pi(i)}, x_j, x_{\pi(j)}) + \text{higher orders.}$$

Review of spatial random permutations

The interaction between jumps $x \mapsto y$ and $x' \mapsto y'$ is

$$V(x,y,x',y') = \int \big[1 - \mathrm{e}{-}\frac{1}{4}\int_0^{4\beta} U(\omega(s))\mathrm{d}s\big]\,\mathrm{d}\widehat{W}^{4\beta}_{x-x',y-y'}(\omega).$$

If U is a hard-core potential with radius a (i.e. $U(r) = \infty$ for $r < a$ and $U(r) = 0$ for $r \geq a$), then $V(\cdot)$ is the probability that a Brownian bridge from $x - x'$ to $y - y'$ hits the ball of radius a centered at the origin.

Is there a simple expression involving special functions? Apparently not.

Review of spatial random permutations: Three models

We simulate three models for spatial random permutations. The first two have been completely coded; the third is in progress.

- The non-interacting model (GRU paper):

$$H(\mathbf{x},\pi) = \frac{1}{4\beta}\sum_{i=1}^{N} \left|x_i - x_{\pi(i)}\right|^2.$$

- The r_2 interacting model (U07 paper):

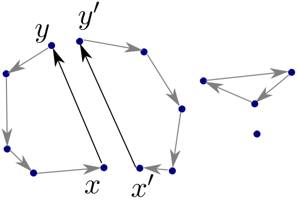
$$H(\mathbf{x},\pi) = \frac{1}{4\beta}\sum_{i=1}^{N} \left|x_i - x_{\pi(i)}\right|^2 + \alpha r_2(\pi).$$

- The interacting model (U07 paper):

$$H(\mathbf{x},\pi) = \frac{1}{4\beta}\sum_{i=1}^{N} \left|x_i - x_{\pi(i)}\right|^2 + \sum_{i<j} V(x_i, x_{\pi(i)}, x_j, x_{\pi(j)}).$$

Review of spatial random permutations: Conceptualization

- The distance-dependent term $e^{-\frac{1}{4\beta}\sum_x \|x-\pi(x)\|^2}$ makes a permutation π with a long jump (i.e. $\pi(x)$ far from x) less probable.
- The $e^{-\alpha r_2(\pi)}$ term discourages permutations with 2-cycles.
- The interacting term discourages permutations with x_i close to x_j and $\pi(x_i)$ close to $\pi(x_j)$, regardless of jump lengths $\|x_i - \pi(x_i)\|$ or $\|x_j - \pi(x_j)\|$. The permutation is favored even less if the two black arrows cross (i.e. larger θ as discussed below).

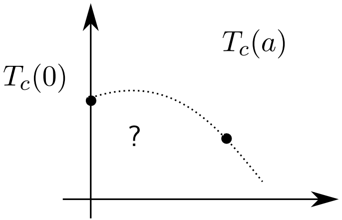


Review of spatial random permutations: Context

The critical temperature T_c for Bose-Einstein condensation is a (mostly unknown) function of scattering length a. Even the sign of the slope of $T_c(a)$ near zero is contested. It is believed that

$$\frac{T_c(a) - T_c(0)}{T_c(0)} = c\rho^{1/d} a + o(\rho^{1/3} a).$$

Currently, it is thought that $c \approx 1.3$. The Monte Carlo simulations described here will permit tighter estimation of c.



Physics literature

1964 Huang: $\frac{\Delta T}{T_c} \sim (a\rho^{1/3})^{3/2}$, increases

1971 Fetter & Walecka: $\frac{\Delta T}{T_c}$ decreases

1982 Toyoda: $\frac{\Delta T}{T_c}$ decreases

1992 Stoof:

$$\frac{\Delta T}{T_c} = c\, a\rho^{1/3} + o(a\rho^{1/3}), \quad c > 0$$

1996 Bijlsma & Stoof: $c = 4.66$

1997 Grüter, Ceperley, Laloë: $c = 0.34$

1999 Holzmann, Grüter, Laloë: $c = 0.7$; Holzmann, Krauth: $c = 2.3$;
Baym et. al.: $c = 2.9$

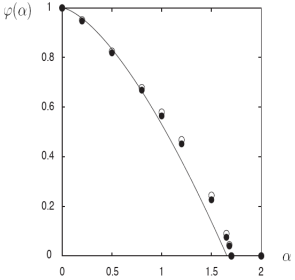
2000 Reppy et. al.: $c = 5.1$

2001 Kashurnikov, Prokof'ev, Svistunov: $c = 1.29$;
Arnold, Moore: $c = 1.32$

2004 Kastening: $c = 1.27$; Nho, Landau: $c = 1.32$

Review of spatial random permutations: Critical temperature

At the critical temperature α, $\phi(\alpha)$ goes to zero. We define $\phi(\alpha)$ to be the probability that the origin is in an infinite cycle. (Here, $\alpha = 1/4\beta$; this figure is from the GRU paper.) Monte Carlo simulations undertaken in this project will discover how this graph changes in the presence of interactions.



The computational project

The computational project

Given a random variable $\theta(\pi)$, compute its expected value. The random variable of interest for this project is the density of site in cycles of specified length:

$$\rho_{mn}(\pi) = \frac{1}{V} \# \left\{ i = 1, \ldots, N : m \leqslant \ell_i(\pi) \leqslant n \right\}$$

The usual prescription in probability is

$$E[\rho_{mn}] = \sum_{\pi \in \mathcal{S}_N} \rho_{mn}(\pi) P(\pi) = \sum_{\pi \in \mathcal{S}_N} \rho_{mn}(\pi) \frac{e^{-H(\mathbf{x},\pi)}}{Y}.$$

The computational project

The computational burden splits into three main components:

(1) Finding H, especially its V term. (For Metropolis, ΔH including ΔV.)

(2) Sampling (via Metropolis) from a non-uniform probability distribution on $N!$ permutations for N as big as 50^3.

(3) Visualizing the results.

Visualization

Visualization

One of my colleagues says "Don't make it a mystery novel." So, I'll show you the pictures first. There are two main plots:

(1) Dot plots of the cycles.

(2) $E[\rho_{0,k}]$ as a function of k from 0 to N.

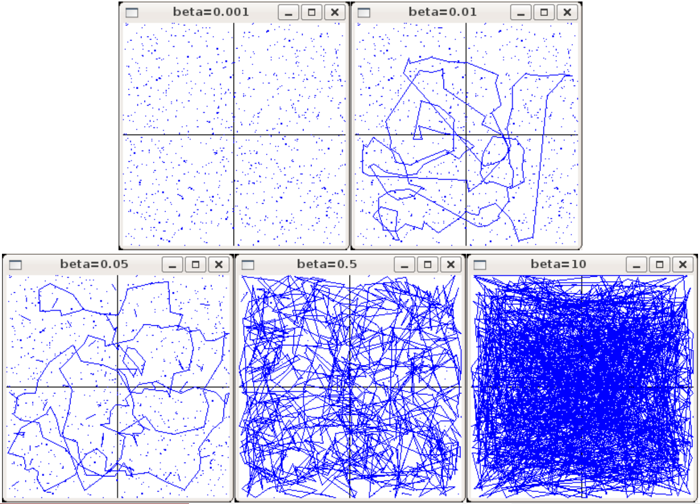
A *dot plot* of the points $\{x_1, \ldots, x_N\}$ and a permutation π has a dot for each point x, along with a line from x to $\pi(x)$ for each point x.

Key points:

- For infinite β, the permutation weight $e^{-\frac{1}{4\beta}\sum_x \|x-\pi(x)\|^2}$ becomes uniform: individual permutation jumps can be arbitrarily long.
- For $\beta = 0$, only the identity permutation is possible.
- For moderate β, long jumps are discouraged. Nonetheless, a long cycle can occur when short jumps chain together.

Visualization: Dot plots, non-interacting case

Here is $L = 10$, $d = 3$, point positions uniformly distributed on the cube of width 10 but not metropolized, no interactions, varying β:



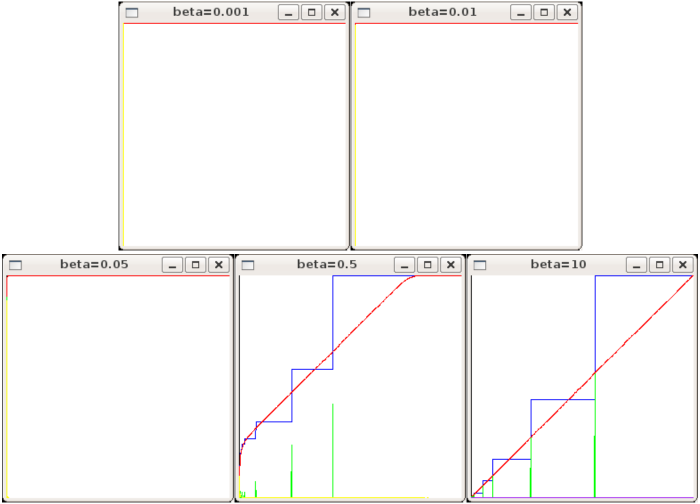
Visualization: $E[\rho]$ plots, non-interacting case

The $E[\rho]$ plots are much as in the GRU paper.

- The horizontal axis is k/N for k from 0 to N.
- In blue on the vertical axis is $\rho_{0,k}$ for the permutation realized on the last Metropolis sweep.
- In green on the vertical axis is $\rho_{k,k}$ for the permutation realized on the last Metropolis sweep.
- In red on the vertical axis is $E[\rho_{0,k}]$ over 10,000 Metropolis sweeps.
- In yellow on the vertical axis is $E[\rho_{k,k}]$.

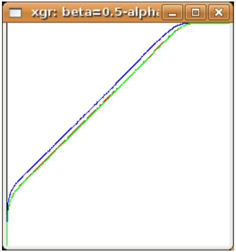
Visualization: $E[\rho]$ plots, non-interacting case

Here are $E[\rho]$ plots for the same parameter values as the dot plots:



Visualization: Plots, r_2 case

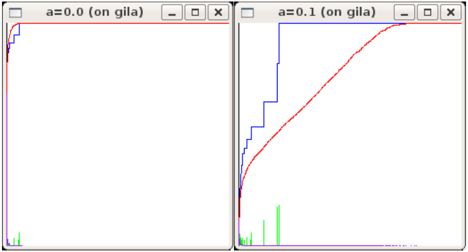
Here we fix $\beta = 0.5$ and vary α. Note that $\alpha = 0$ recovers the non-interacting case. The dot plots are indistinguishable. The $E[\rho_{0,k}]$ plots are similar, so they are superimposed. Blue is $\alpha = 0$, red is $\alpha = 5$, and green is $\alpha = 20$.



Visualization: $E[\rho]$ plots, interacting case

This is recent work — more are to be obtained.

Here is $\beta = 0.15626$ (just below non-interacting critical temperature), with $a = 0.0$ and $a = 0.1$:



Comparison

The value $\phi(\beta)$ is the probability that the origin is in an "infinite" cycle. It may be read off the $E[\rho]$ plots as the distance from the upper left corner of the ρ plot to the first leftward lean of the red curve. Critical β_c has $\phi(\beta) = 0$.

β	$\phi_0(\beta)$	$\phi_{\alpha=4}(\beta)$	$\phi_{a=0.1}(\beta)$
0.227273	0.5203	0.5824	0.8081
0.208333	0.4373	0.5114	0.8057
0.192308	0.3703	0.4440	0.7835
0.178571	0.2625	0.3097	0.7868
0.166667	0.1517	0.2148	0.7769
0.161290	0.1133	0.1637	0.7663
0.156250	0.0824	0.1220	0.7693
0.147059	0.0311	0.0351	0.7645

Conclusion: interactions lower critical β. More simulations are needed.

Computation of V

Computation of V: Brownian bridges

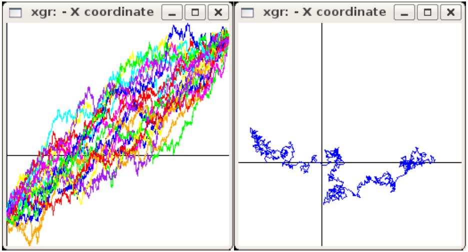
Write $\hat{x}$ and $\hat{y}$ for $x - x'$ and $y - y'$ respectively. Simply generate N_b Brownian bridges from $\hat{x}$ to $\hat{y}$, with N_p mesh points per bridge, and see what fraction of them intersects the ball of radius a centered at the origin.

- Start with a unit-uniform pseudorandom number generator (RNG).
- Use a Box-Muller transform (cf. *Numerical Recipes*) to get standard-normal deviates.
- Brownian motion for t from 0 to 1 in steps of Δt: $B_0 = 0$ and $B_{t+1} = B_t + \Delta B$ where ΔB is normal with mean zero and variance Δt.
- Brownian bridge from $\hat{x} = 0$ to $\hat{y} = 0$ for t from 0 to 1: $R_t = B_t - tB_1$.
- Brownian bridge from $\hat{x}$ to $\hat{y}$ for t from 0 to T: $\sqrt{T}R_t + \hat{x} + \frac{t}{T}(\hat{y} - \hat{x})$.

Computation of V: Brownian bridges

The plot on the left shows, for $d = 1$, $N_b = 20$ bridges with $N_p = 1000$ points per bridge, bridged from $x = -1$ to $y = 2$ $(d = 1)$ in time $T = 1$, with R_t plotted against t.

The plot on the right shows, for $d = 3$, the trajectory of a single bridge from $x = (-1, 0, 0)$ to $y = (2, 0, 0)$ in time $T = 1$, with the first two components of R_t plotted.



Computation of V: Brownian bridges

Experimental results are discouraging. Performance requirements are too stiff for generation of Brownian bridges during Metropolis steps. To help this, one can (1) compute a database of zero-to-zero N_b Brownian bridges of N_p points each, and re-use this database for different $\hat{x}, \hat{y}$. (2) Tabulate V off-line and interpolate at runtime.

- Dependence on N_b: Increasing N_b decreases sampling variability of V.
- Dependence on N_p: For small N_p, increasing N_b only decreases sampling variablity, but non-zero bias remains (vs. the integral and exact expressions, shown next). For the test case $r_1 = 1$, $r_2 = 1$, $\theta = \pi$, one needs N_p on the order of 500,000 before V begins to stabilize.

Interpretation: Note that $\Delta t = T/N_p$. Standard deviation of bridge steps is on the order of $\sqrt{T/N_p}$. For smaller N_p, bridges are too “hoppy” and miss the a-ball at the origin.

Computation of V: Integral expression

Ueltschi and Betz have recently found an approximation which is valid to low order in a:

$$V_2(\hat{x},\hat{y}) = \frac{a}{\sqrt{8\pi\beta}} e^{\frac{+\|\hat{x}-\hat{y}\|^2}{8\beta}} \int_0^1 \frac{1}{[s(1-s)]^{3/2}} e^{-\frac{\|\hat{x}\|^2}{8\beta s}} e^{-\frac{\|\hat{y}\|^2}{8\beta(1-s)}} \mathrm{d}s.$$

where, for notational convenience, we write

$$\hat{x} = x - x', \quad \hat{y} = y - y', \quad V_2(\hat{x},\hat{y}) = V(x,y,x',y').$$

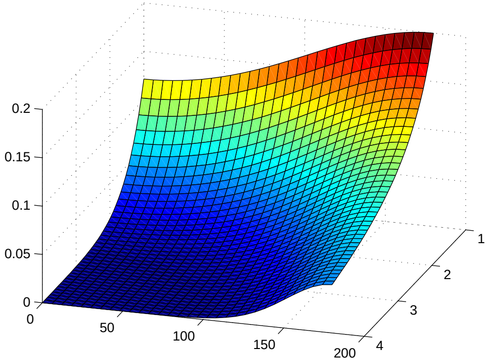
If $\|\hat{x}\| = \|\hat{y}\|$ then we have the exact expression

$$V_2(\hat{x},\hat{y}) = \frac{2a}{\|\hat{x}\|} e^{\frac{+\|\hat{x}-\hat{y}\|^2}{8\beta}} e^{\frac{-\|\hat{x}\|^2}{2\beta}}.$$

This can be written in terms of the five real variables $r_1 = \|x\|$, $r_2 = \|y\|$, $\theta = \cos^{-1}(\langle x,y\rangle / \|x\|\,\|y\|)$, β, and a.

Computation of V: Visualization

Here is a surface plot of $V(r, r, \theta)$ for r from 1 to 4, θ from 0 to π, $\beta = 1$, and $a = 0.1$. Note that probability of intersecting the a-sphere decays as r increases, and grows as θ runs from 0° to 180°, as expected.



Conclusions and further directions

Conclusions

- The r_2 model is easy to simulate. The r_2 term raises the critical temperature. One can quantify this dependence and verify it against the result of Betz and Ueltschi.
- Preliminary results show that in the full-interaction model, the critical temperature is also raised. Software optimization is currently in progress, so that more simulations may be done in a timely manner. Then, $T_c(a)$ may be plotted with confidence.

Further directions

- The cluster expansion is non-rigorous and needs further justification, in particular for non-lattice point distributions where inter-particle spacing can be small.
- Examine random variables other than ρ_{mn}.
- Use non-Gaussian weights for $d = 2$.
- Place the points not on a cubic lattice but distributed according to a point process; metropolize point positions as well as permutations. The correct point process for Bose-Einstein condensation is not known; it is known *not* to be Poisson.
- We can greatly increase system size by using parallelization: on a multiprocessor system, partition Λ into subcubes. When x, y are in the same subcube, computation is local; when x is in one subcube and y is in a neighbor, use message-passing.
- See what people come up with as $T_c(a)$ becomes better known .... Stay tuned for this as well!