Worm portion of dissertation (rough draft)

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1 Disclaimer

These are rough notes for the portion of my dissertation relating to the RCM worm algorithm.

2 The random-cycle model and the GRU algorithm

2.1 The random-cycle model

We have N points $\mathbf{x}_1, \ldots, \mathbf{x}_N$ in a cube $[0, L]^d$ in $\mathbb{R}^d$ (nominally, $d = 3$) with periodic boundary conditions. For $\pi \in \mathcal{S}_N$, we have **energy functions**

$$H(\pi) = \frac{1}{4\beta} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{\ell=2}^{N} \alpha_\ell N_\ell(\pi) \qquad \text{(cycle weights)} \tag{2.1.1}$$

or

$$H(\pi) = \frac{1}{4\beta} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{i<j} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) \qquad \text{(jump-pair interactions).} \tag{2.1.2}$$

Remark 2.1.3. We should write $H(\mathbf{x}_1, \ldots, \mathbf{x}_N, \pi)$. However, either we work on a lattice where the $\mathbf{x}_i$'s are held fixed, or on the continuum where the $\mathbf{x}_i$'s are integrated out.

Remark 2.1.4. For jump-pair interactions, the arrow $\mathbf{x}_i \mapsto \mathbf{x}_{\pi(i)}$ interacts with the arrow $\mathbf{x}_j \mapsto \mathbf{x}_{\pi(j)}$.

Definition 2.1.5. At present we restrict attention to the lattice points $\mathcal{L}$:

$$\mathcal{L} = [0, L]^d \cap \mathbb{Z}^d.$$

Note that there are $N = L^d$ lattice sites.

From either of these energy functions we define a **probability density** on $\mathcal{S}_N$ via a **Gibbs distribution**:

$$P(\pi) = \frac{e^{-H(\pi)}}{Z} \tag{2.1.6}$$

where the **partition function** is

$$Z = \sum_{\pi \in \mathcal{S}_N} e^{-H(\pi)}. \tag{2.1.7}$$

Definition 2.1.8. Fixing $\pi \in \mathcal{S}_N$, for $\mathbf{x} \in \mathcal{L}$, $\ell_\pi(\mathbf{x})$ (or simply $\ell(\mathbf{x})$) is the smallest positive number a such that $\pi^a(\mathbf{x}) = \mathbf{x}$. This is the length of the cycle containing $\mathbf{x}$.

2.2 The GRU algorithm

The **GRU algorithm** for sampling from this distribution is as follows:

- Start with the identity or uniform-random permutation.

- Sweep through sites $\mathbf{x}$ of the lattice in either lexical or uniform-random order.
- For each site $\mathbf{x}$, do a **Metropolis step**:
  - Choose a site $\pi(\mathbf{y})$ from among the six nearest neighbors of $\pi(\mathbf{x})$.
  - Propose to change π to the permutation π' which has $\pi'(\mathbf{z}) = \pi(\mathbf{z})$ for all $\mathbf{z} \neq \mathbf{x}, \mathbf{y}$ but $\pi'(\mathbf{x}) = \pi(\mathbf{y})$ and $\pi'(\mathbf{y}) = \pi(\mathbf{x})$. (See figure 1.)
  - With probability proportional to $\min\{1, e^{-\Delta H}\}$ where $\Delta H = H(\pi') - H(\pi)$, accept the change. (If the change is rejected, $\pi' = \pi$.)
- After each sweep[1], obtain a value of random variable(s) for inclusion in computation of their sample means.

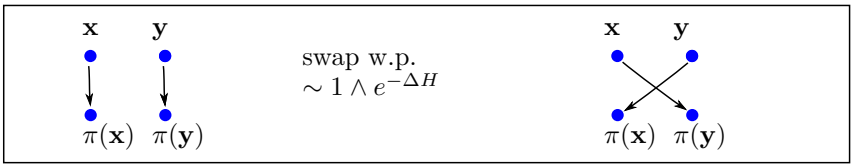

Figure 1: Metropolis moves for the GRU algorithm.

Definition 2.2.1. A GRU swap is **trivial** if $\mathbf{x} = \mathbf{y}$.

2.3 Explicit construction of the Markov matrix

For section 2.4 we will need an explicit construction of the Markov matrix corresponding to the GRU algorithm as described in section 2.2.

The Markov perspective on the algorithm is that the distribution $P^{(0)}(\pi)$ of the first permutation is either supported solely on the identity, or uniform on all $N!$ permutations. The distribution for subsequent permutations is

$$P^{(k+1)}(\pi') = \sum_{\pi \in \mathcal{S}_N} P^{(k)}(\pi) M(\pi, \pi')$$

or, in matrix/vector notation,

$$\mathbf{P}^{(k+1)} = \mathbf{P}^{(k)} \mathbf{M}.$$

In this section we precisely describe the matrix $\mathbf{M}$; in section 2.4 we show that $\mathbf{P}^{(k)}$ approaches the Gibbs distribution (equation 2.1.6).

The matrix $\mathbf{M}$ is $N! \times N!$: rows are indexed by $\pi_1, \ldots, \pi_{N!}$ and columns are indexed by $\pi'_1, \ldots, \pi'_{N!}$. Most of the entries of $\mathbf{M}$ are zero: Metropolis steps change only two permutation sites whereas most π, π' differ at more than two sites.

Definition 2.3.1. For $\pi, \pi' \in \mathcal{S}_N$, define

$$d(\pi, \pi') = \#\{i = 1, 2, \ldots, N : \pi(i) \neq \pi'(i)\}.$$

[1]Or after a specified number of sweeps. This choice depends on autocorrelation time, which is beyond the scope of this section.

Remark. Note that $d(\pi, \pi') \neq 1$ since if two permutations agree on $N-1$ sites, they must agree on the remaining site.

Lemma 2.3.2. *The function $d(\pi, \pi')$ is a metric on $\mathcal{S}_N$.*

Proof. Symmetry is obvious, as is non-negativity. For positive definiteness, note that $d(\pi, \pi') = 0$ iff $\pi = \pi'$. For the triangle inequality, let $\pi, \pi', \pi'' \in \mathcal{S}_N$. Partition the set $\{1, 2, \ldots, N\}$ into the four disjoint sets

$$\begin{aligned}
A &= \{i = 1, 2, \ldots, N : \pi(i) = \pi'(i), \pi'(i) = \pi''(i)\}, \\
B &= \{i = 1, 2, \ldots, N : \pi(i) = \pi'(i), \pi'(i) \neq \pi''(i)\}, \\
C &= \{i = 1, 2, \ldots, N : \pi(i) \neq \pi'(i), \pi'(i) = \pi''(i)\}, \\
D &= \{i = 1, 2, \ldots, N : \pi(i) \neq \pi'(i), \pi'(i) \neq \pi''(i)\}.
\end{aligned}$$

Then $\pi = \pi''$ on all of A; $\pi \neq \pi''$ on all of B and C; and π, π'' may or may not agree on various elements of D:

A	B	C	D
$\pi = \pi'$	$\pi = \pi'$	$\pi \neq \pi'$	$\pi \neq \pi'$
$\pi' = \pi''$	$\pi' \neq \pi''$	$\pi' = \pi''$	$\pi' \neq \pi''$
$\pi = \pi''$	$\pi \neq \pi''$	$\pi' \neq \pi''$	Varies

That is,

$$\begin{aligned}
d(\pi, \pi') &= \#C + \#D, \\
d(\pi', \pi'') &= \#B + \#D, \\
\#B + \#C \leq d(\pi, \pi'') &\leq \#B + \#C + \#D.
\end{aligned}$$

Then

$$d(\pi, \pi'') \leq \#B + \#C + \#D \leq \#B + \#C + 2\#D = d(\pi, \pi') + d(\pi', \pi'').$$

□

Definition 2.3.3. Lattice sites $\mathbf{x}, \mathbf{y}$ are **nearest-neighbor** if $\|\mathbf{x} - \mathbf{y}\| = 1$.

Definition 2.3.4. For $\pi \in \mathcal{S}_N$, define

$$R(\pi) = \{\pi' \in \mathcal{S}_N : d(\pi, \pi') = 2 \text{ and } \|\pi(\mathbf{x}) - \pi(\mathbf{y})\| = 1\}$$

where the $\mathbf{x}$ and $\mathbf{y}$ are taken to be the two points at which π, π' differ. Then $R(\pi)$ is the set of permutations π' reachable from π on a GRU swap.

The Metropolis steps are then described as follows. For each $\pi \in \mathcal{S}_N$,

$$M(\pi, \pi') = \begin{cases} C\left(1 \wedge e^{-H(\pi') + H(\pi)}\right), & \pi' \in R(\pi), \\ 1 - \displaystyle\sum_{\pi' \in R(\pi)} C\left(1 \wedge e^{-H(\pi') + H(\pi)}\right), & \pi = \pi'; \\ 0, & \text{otherwise.} \end{cases}$$

To find out what C is:

- There are N choices of lattice points $\mathbf{x}$.

- For each $\mathbf{x}$, there are 6 choices of $\pi(\mathbf{y})$ which are nearest neighbors to $\pi(\mathbf{x})$.
- This double-counts the $3N$ distinct choices of π' reachable from π in a single Metropolis step, since choosing $\mathbf{x}$ and then $\mathbf{y}$ results in the same Metropolis step as choosing $\mathbf{y}$ and then $\mathbf{x}$.

We require rows sums to be 1 for stochastic matrices so we may take

$$C = \frac{1}{3N}.$$

This prefactor of $1/3N$ is the same for all non-zero entries of $\mathbf{M}$ for GRU Metropolis. Then

$$M(\pi, \pi') = \begin{cases} \frac{1}{3N}\left(1 \wedge e^{-H(\pi')+H(\pi)}\right), & \pi' \in R(\pi), \\ 1 - \sum_{\pi' \in R(\pi)} C\left(1 \wedge e^{-H(\pi')+H(\pi)}\right), & \pi = \pi'; \\ 0, & \text{otherwise.} \end{cases} \tag{2.3.5}$$

2.4 Correctness of the GRU algorithm

It is clear that the GRU algorithm produces a sequence of permutations, but with what distribution? From Markov-chain theory, we know the following: If the chain is irreducible, aperiodic, and satisfies detailed balance, then the chain has the Gibbs distribution (equation 2.1.6) as its unique invariant distribution.

Terminology: **detailed balance** is the same as **reversibility**. Also, an irreducible, aperiodic chain on a finite state space is called **ergodic**.

Also note from Markov-chain theory that all states in a recurrence class have the same period. Thus, if we can show that the chain is irreducible (i.e. the entire state space is a single recurrence class), then for aperiodicity of the chain it suffices to show that a single state (e.g. the identity permutation) has period 1.

Proposition 2.4.1 (Irreducibility)**.** *For all π, π', there is an n such that $M^n(\pi, \pi') > 0$. That is, any permutation is reachable from any other.*

Proof. This non-trivial result needs to be proved. □

Remark. Below we will discuss winding cycles, and the empirical fact that the GRU algorithm reaches them only rarely. The chain is irreducible but the non-zero transition probability can still be very small.

Definition 2.4.2. A permutation π has period p if any return to π must occur at multiples of p steps. Precisely, let Π_n be the random variable which is the nth value of the Markov chain. Then

$$p = \gcd\{n : P(\Pi_n = \pi \mid \Pi_0 = \pi) > 0\}.$$

Furthermore, the chain is said to be aperiodic if all states are aperiodic.

Proposition 2.4.3 (Aperiodicity)**.** *The GRU algorithm's Markov chain is aperiodic.*

Proof. From Markov-chain theory, we know that all states in a recurrence class have the same period. Thus, it suffices to show that one state, e.g. the identity, is aperiodic. If there is non-zero probability of transitioning from the identity to itself, the identity is an aperiodic state. But this in fact the case: The identity has zero energy (equations 2.1.1, 2.1.2). Any state proposed as a transition from the identity is necessarily a two-cycle, for which the distance terms in equation 2.1.1,2.1.2 are positive. The cycle-weight terms or interaction terms are non-negative. Thus $\Delta H > 0$, and the GRU Metropolis transition probability is strictly less than 1. Therefore there is a non-zero probability of staying at the identity permutation. □

Proposition 2.4.4 (Detailed balance)**.** *For all* $\pi, \pi' \in \mathcal{S}_N$*,*

$$P(\pi)M(\pi,\pi') = P(\pi')M(\pi',\pi). \tag{2.4.5}$$

Proof. The detailed-balance statement in terms of the Gibbs distribution (equation 2.1.6) and the GRU Metropolis transition matrix (equation 2.3.5) is

$$\frac{e^{-H(\pi)}}{Z}\left(1 \wedge e^{-H(\pi')}e^{H(\pi)}\right) \stackrel{?}{=} \frac{e^{-H(\pi')}}{Z}\left(1 \wedge e^{-H(\pi)}e^{H(\pi')}\right).$$

The Z's cancel. The lemma below shows that $M(\pi,\pi') \neq 0$ iff $M(\pi',\pi) \neq 0$. If $M(\pi,\pi') = 0$, then detailed balance holds. If $M(\pi,\pi') \neq 0$, then there are two cases. If $H(\pi') \leq H(\pi)$, then

$$e^{-H(\pi)}(1) = e^{-H(\pi')}\left(e^{-H(\pi)}e^{H(\pi')}\right).$$

If $H(\pi') > H(\pi)$,

$$e^{-H(\pi)}\left(e^{-H(\pi')}e^{H(\pi)}\right) = e^{-H(\pi')}(1).$$

In all cases, detailed balance holds. □

Lemma 2.4.6. *For all* $\pi, \pi' \in \mathcal{S}_N$*,*

$$M(\pi,\pi') \neq 0 \iff M(\pi',\pi) \neq 0.$$

Proof. If $d(\pi,\pi') > 2$, then $M(\pi,\pi') = 0$ and $M(\pi',\pi) = 0$.

If $d(\pi,\pi') = 2$, then π and π' differ at two sites $\mathbf{x}$ and $\mathbf{y}$. Put

$$\begin{aligned} \pi(\mathbf{x}) &= \mathbf{u}, & \pi'(\mathbf{x}) &= \mathbf{v}, \\ \pi(\mathbf{y}) &= \mathbf{v}, & \pi'(\mathbf{y}) &= \mathbf{u}. \end{aligned}$$

If $\|\mathbf{u} - \mathbf{v}\| = 1$ then $M(\pi,\pi') \neq 0$ and $M(\pi',\pi) \neq 0$ since $\mathbf{u}$ and $\mathbf{v}$ are nearest-neighbor lattice sites. If $\|\mathbf{u} - \mathbf{v}\| > 1$ then $M(\pi,\pi') = 0$ and $M(\pi',\pi) = 0$ since $\mathbf{u}$ and $\mathbf{v}$ are not nearest-neighbor lattice sites.

Last, if $\pi = \pi'$, then $M(\pi,\pi') = M(\pi',\pi)$. □

This lemma completes the proof that the GRU algorithm satisfies detailed balance and thus has the Gibbs distribution as its invariant distribution.

The following proposition is not a correctness result, but rather a sanity check. It shows that cycles may grow or shrink upon GRU moves.

Figure 2: GRU swaps merge disjoint cycles and split single cycles. The left-hand permutation can be reached from the right-hand permutation via a GRU swap, and vice versa.

Proposition 2.4.7. *If* $\mathbf{x}$ *and* $\mathbf{y}$ *are in disjoint cycles before a non-trivial GRU swap then they are in the same cycle afterward and vice versa (see figure 2).*

Proof. First suppose that $\mathbf{x}$ and $\mathbf{y}$ are in disjoint cycles. Let the respective cycle lengths be $\ell(\mathbf{x}) = a$ and $\ell(\mathbf{y}) = b$. Those cycles are

$$\mathbf{x} \mapsto \pi(\mathbf{x}) \mapsto \pi^2(\mathbf{x}) \mapsto \ldots \mapsto \pi^{a-1}(\mathbf{x}) \mapsto \mathbf{x} \quad \text{and} \quad \mathbf{y} \mapsto \pi(\mathbf{y}) \mapsto \pi^2(\mathbf{y}) \mapsto \ldots \mapsto \pi^{b-1}(\mathbf{y}) \mapsto \mathbf{y}.$$

Since these are disjoint cycles, all elements listed are distinct lattice sites. After the swap, we have

$$\mathbf{y} \mapsto \pi(\mathbf{x}) \mapsto \pi^2(\mathbf{x}) \mapsto \ldots \mapsto \pi^{a-1}(\mathbf{x}) \mapsto \mathbf{x} \quad \text{and} \quad \mathbf{x} \mapsto \pi(\mathbf{y}) \mapsto \pi^2(\mathbf{y}) \mapsto \ldots \mapsto \pi^{b-1}(\mathbf{y}) \mapsto \mathbf{y}.$$

This is a single cycle of length $a + b$, starting with $\mathbf{y}$, including $\mathbf{x}$, and returning to $\mathbf{y}$.

Second, suppose that $\mathbf{x}$ and $\mathbf{y}$ are in the same cycle. Let a be the smallest positive integer such that $\pi^a(\mathbf{x}) = \mathbf{y}$; let b be the smallest positive integer such that $\pi^b(\mathbf{y}) = \mathbf{x}$. (These numbers are both positive since the swap is non-trivial, i.e. $\mathbf{x} \neq \mathbf{y}$.) Then we have

$$\mathbf{x} \mapsto \pi(\mathbf{x}) \mapsto \pi^2(\mathbf{x}) \mapsto \pi^{a-1}(\mathbf{x}) \mapsto \mathbf{y} \mapsto \pi(\mathbf{y}) \mapsto \pi^2(\mathbf{y}) \mapsto \ldots \mapsto \pi^{b-1}(\mathbf{y}) \mapsto \mathbf{x}.$$

This is a single cycle of length $a + b$; all lattice sites listed are distinct. After the swap, we have

$$\mathbf{y} \mapsto \pi(\mathbf{x}) \mapsto \pi^2(\mathbf{x}) \mapsto \pi^{a-1}(\mathbf{x}) \mapsto \mathbf{y} \quad \text{and} \quad \mathbf{x} \mapsto \pi(\mathbf{y}) \mapsto \pi^2(\mathbf{y}) \mapsto \ldots \mapsto \pi^{b-1}(\mathbf{y}) \mapsto \mathbf{x}.$$

These are disjoint cycles of length a and b, respectively; the first contains $\mathbf{x}$ and the second contains $\mathbf{y}$. □

3 The random-cycle model and the worm algorithm

Here an alternative to the GRU algorithm is motivated and proved correct.

3.1 Winding cycles

Recall that we have permutations on $[0, L]^3$ with periodic boundary conditions. Topologically, this is a 3-torus. Permutation cycles may wind around the 3-torus some number of times in the x, y, and/or z directions. If a cycle goes around once in the clockwise direction, we want to say it has sign $+1$; likewise, we want sign -1 for the counterclockwise direction. The following definition formalizes this intuition.

Definition 3.1.1. The **winding number W** of a permutation is the triple of integers

$$\mathbf{W} = (W_x, W_y, W_z) = \frac{1}{L} \sum_{i=1}^{N} (\mathbf{x}_{\pi(i)} - \mathbf{x}_i).$$

We also write

$$\mathbf{W}^2 = \mathbf{W} \cdot \mathbf{W} = W_x^2 + W_y^2 + W_z^2.$$

It is found empirically with the GRU algorithm that winding cycles are created with opposite signs, such that permutations have winding number zero. E.g. there might be a cycle with $W_x = 1$ and another cycle with $W_x = -1$. The same problem is observed in PIMC studies. (References TBD.)

One solution is to modify the GRU algorithm to reverse, with probability 1/2, the direction of arrows in modified cycles. This is a partial remedy: it results in permutations with even winding numbers.

The **superfluid fraction** is [cite PC87]

$$f_S = \frac{\langle \mathbf{W}^2 \rangle L^2}{3\beta N} = \frac{\langle \mathbf{W}^2 \rangle}{3\beta L}.$$

We use this as an order parameter with which to detect the critical temperature.

3.2 PIMC motivation

Say something here about PIMC, worldlines, and the gist of the PIMC worm algorithm. Mention the grand-canonical ensemble. References TBD.

[figures here]

3.3 Idea of the worm algorithm

The key selling point of the random-cycle model is that Brownian bridges have been integrated out. Most of the complexity of PIMC simulations goes away. If I want to adapt a PIMC worm algorithm to the RCM, I need to spend a lot of my time learning about PIMC, but probably ultimately most of the complexity will also go away. Instead, it is simpler to ask: If we were to have a worm algorithm for the random-cycle model, what properties would it have? We require the following:

- We have a lattice with a fixed number N of points. There is no desire to work in the grand-canonical ensemble.
- We want the ability to open and close permutation cycles. (An open cycle is a "worm".)
- Given that, tips of open cycles may wander around the 3-torus before closing, permitting arbitrary winding numbers.

Idea: sometimes open a cycle, then modify it with GRU-like steps, then close it again. Following PIMC worm, all Metropolis steps involve the worm. This does touch all lattice points: a worm is opened at a site, then modified, then closed. Then, a worm is opened somewhere else, and so on.

Question: Can we leverage our knowledge of permutations?

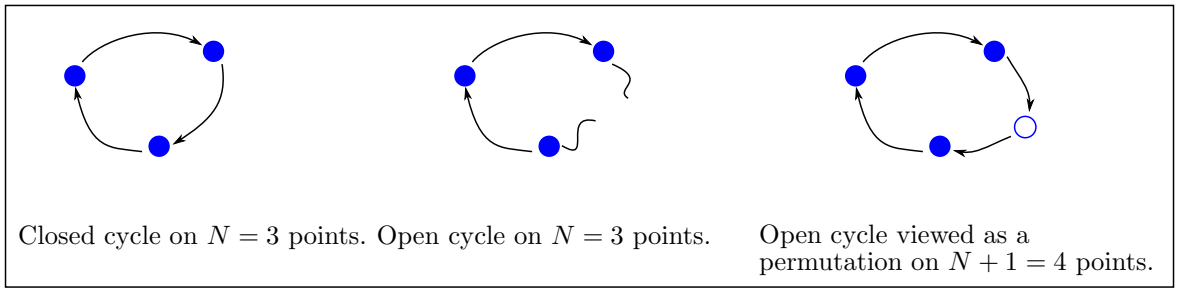

Figure 3: Open cycles as permutations on $N + 1$ points.

Closed cycle:

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}$$

Open cycle:

$$\begin{pmatrix} 1 & 2 & 3 & \\ 2 & 3 & & 1 \end{pmatrix}$$

Here, $1 \mapsto 2$, $2 \mapsto 3$, $3 \mapsto$ nothing, and nothing $\to 1$. Call that nothing *something* — the **wormhole point**. It is an $(N + 1)$st point:

$$\begin{pmatrix} 1 & 2 & 3 & w \\ 2 & 3 & w & 1 \end{pmatrix}$$

Henceforth, the wormhole point will be written as w or $N + 1$. In diagrams, it will be an open dot while the other N points will be written with filled dots. (See figure 3.)

Now we have permutations on $\mathcal{S}_{N+1}$. Given $\pi \in \mathcal{S}_N$, inject π into $\mathcal{S}_{N+1}$ via $\pi(w) = w$.

Definition 3.3.1. For $\pi \in \mathcal{S}_{N+1}$, we say π is a **closed permutation** if $\pi(w) = w$. We say π is an **open permutation** if $\pi(w) \neq w$. Likewise, a cycle of π is open or closed, respectively, if it does or does not contain w.

Remark. The PIMC jargon is that closed permutations are in the *Z sector* (for partition function), while open permutations are in the *G sector* (for Matsubara Green's function).

The goal is to invent an energy function, Gibbs distribution, and Metropolis algorithm for these extended permutations in $\mathcal{S}_{N+1}$ such that the marginal distribution on $\mathcal{S}_{N+1}$, conditioned on closed permutations, matches the RCM Gibbs distribution (equation 2.1.6). Then, random variables will be sampled only at closed permutations.

3.4 Extended random-cycle model

Recall that we inject $\pi \in \mathcal{S}_N$ into $\mathcal{S}_{N+1}$ via $\pi(w) = w$. The $(N+1)$st point w is **non-spatial**: it has no distance associated with it.

Definition 3.4.1. The **extended lattice** is

$$\mathcal{L}' := \mathcal{L} \cup \{w\}$$

Definition 3.4.2. For $\pi \in \mathcal{S}_{N+1}$, define

$$H'(\pi) = \frac{1}{4\beta} \sum_{\substack{i=1 \\ \pi(\mathbf{x}_i) \neq w}}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{\ell=2}^{N} \alpha_\ell N_\ell(\pi) + \gamma 1_{\mathcal{S}_{N+1} \setminus \mathcal{S}_N}(\pi). \tag{3.4.3}$$

Note that this **extended energy** agrees with the RCM energy (equation 2.1.1) on closed permutations. This is used to prove the marginality condition below.

A small positive γ factor is sufficient to establish aperiodicity of the Markov chain (proposition 3.9.4).

The **extended Gibbs distribution** and **extended partition function** are defined in the obvious way.

Definition 3.4.4. Let

$$P'(\pi) = \frac{e^{-H'(\pi)}}{Z'} \tag{3.4.5}$$

where the partition function is

$$Z' = \sum_{\pi \in \mathcal{S}_{N+1}} e^{-H'(\pi)}. \tag{3.4.6}$$

3.5 Proof of marginality

As long as the energy function for the ERCM and the RCM agree on closed permutations, the desired marginality condition holds. This means that either of the interactions in 2.1.1 or 2.1.2 — or any other to-be-invented interaction models — may use the worm algorithm as long as they agree on closed permutations.

Proposition 3.5.1 (Marginality condition)**.** *Let $\mathcal{S}_N \hookrightarrow \mathcal{S}_{N+1}$ by taking $\pi(w) = w$. Let H, H' be energy functions on $\mathcal{S}_N$ and $\mathcal{S}_{N+1}$, respectively, such that for all $\pi \in \mathcal{S}_N$,*

$$H(\pi) = H'(\pi). \tag{3.5.2}$$

Let P, P', Z, Z' be as above. Then for $\pi \in \mathcal{S}_N$,

$$P'(\pi \mid \pi \in \mathcal{S}_N) = P(\pi). \tag{3.5.3}$$

Proof. Let $\pi \in \mathcal{S}_N$. The left-hand side of equation 3.5.3 is, by definition of conditional expectation,

$$P'(\pi \mid \pi \in \mathcal{S}_N) = \frac{P'(\pi)\ 1_{\mathcal{S}_N}(\pi)}{P'(\mathcal{S}_N)}.$$

The numerator is the Gibbs probability for closed permutations, or zero for open ones:

$$P'(\pi)\ 1_{\mathcal{S}_N}(\pi) = \frac{1}{Z'} e^{-H'(\pi)}\ 1_{\mathcal{S}_N}(\pi) = \frac{1}{Z'} e^{-H(\pi)}\ 1_{\mathcal{S}_N}(\pi)$$

since H and H' agree on closed permutations. The denominator is the total probability of closed permutations:

$$P'(\mathcal{S}_N) = \frac{1}{Z'} \sum_{\pi \in \mathcal{S}_N} e^{-H'(\pi)} = \frac{1}{Z'} \sum_{\pi \in \mathcal{S}_N} e^{-H(\pi)}.$$

Since $\pi \in \mathcal{S}_N$, the ratio is

$$\begin{aligned} \frac{\frac{1}{Z'} e^{-H(\pi)}\ 1_{\mathcal{S}_N}(\pi)}{\frac{1}{Z'} \sum_{\pi \in \mathcal{S}_N} e^{-H(\pi)}} &= \frac{e^{-H(\pi)}\ 1_{\mathcal{S}_N}(\pi)}{\sum_{\pi \in \mathcal{S}_N} e^{-H(\pi)}} \\ &= \frac{e^{-H(\pi)}\ 1_{\mathcal{S}_N}(\pi)}{Z} \\ &= P(\pi). \end{aligned}$$

□

3.6 The worm algorithm

Now that we have the correct Gibbs distribution for the ERCM, the next step is to devise a Metropolis algorithm to sample from it. Below, we will prove correctness.

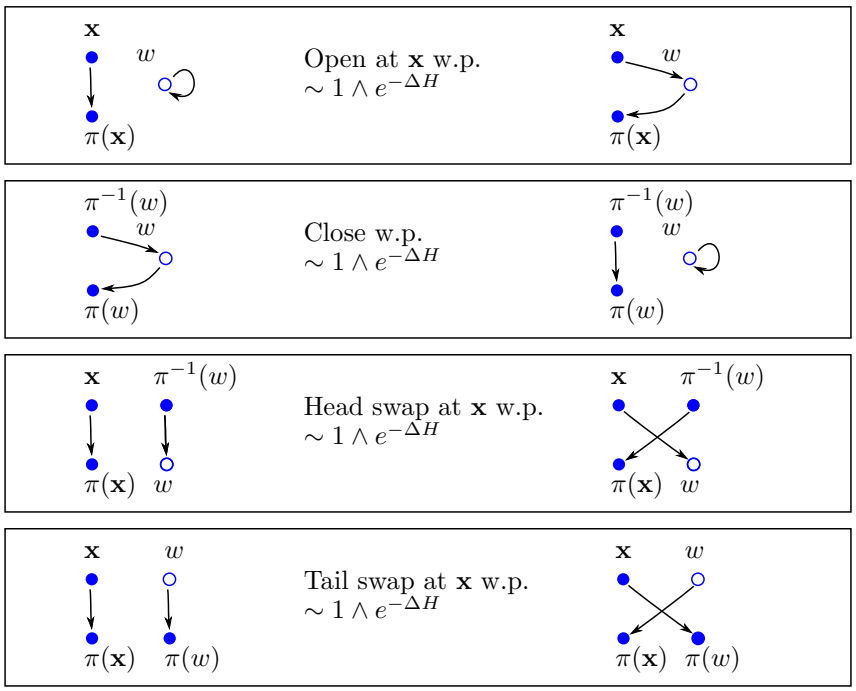

Figure 4: Metropolis moves for the worm algorithm.

The **worm algorithm** is as follows:

- Start with the identity or uniform-random closed permutation.
- The permutation is now closed, so $\pi(w) = w$. Select a lattice site $\mathbf{x}$ at uniform random. With probability proportional to $1 \wedge e^{-\Delta H}$, open the permutation by swapping the arrows of $\mathbf{x}$ and w. This is called an **open** move. (See figure 4.)
- Now that the permutation is open, do a **head swap**, **tail swap**, or **close**.
- Head swap: Pick a lattice site $\mathbf{x}$ nearest-neighbor to the lattice site $\pi^{-1}(w)$. With probability proportional to $1 \wedge e^{-\Delta H}$, swap arrows as in figure 4. The head swap is trivial if $\mathbf{x} = \pi^{-1}(w)$, which happens only if the head swap is rejected. The head swap would be a close if $\mathbf{x} = w$, but we choose $\mathbf{x}$ to be a lattice site. Thus, the permutation remains open on a head swap.
- Tail swap: Pick a lattice site $\pi(\mathbf{x})$ nearest-neighbor to the lattice site $\pi(w)$. With probability proportional to $1 \wedge e^{-\Delta H}$, swap arrows as in figure 4. The tail swap is trivial if $\pi(\mathbf{x}) = \pi(w)$, which happens only if the tail swap is rejected. The tail swap would be a close if $\pi(\mathbf{x}) = w$, but we choose $\pi(\mathbf{x})$ to be a lattice site. Thus, the permutation remains open on a tail swap.
- Close: with probability proportional to $1 \wedge e^{-\Delta H}$, swap arrows as in figure 4. The permutation is now closed.
- Once the permutation is closed — after an open, some number of head/tail swaps, and a close, or after a rejected open — a **worm sweep** has been completed. At every sweep (or after every specified number of sweeps as noted in the autocorrelation footnote above), one may obtain a value of random variable(s) for inclusion in computation of their sample means.

Definition 3.6.1. A head swap at $\mathbf{x}$ is **trivial** if $\mathbf{x} = \pi^{-1}(w)$; a tail swap at $\mathbf{x}$ is trivial if $\pi(\mathbf{x}) = \pi(w)$.

3.7 Fibration of $\mathcal{S}_{N+1}$ over $\mathcal{S}_N$

The definitions and lemmas in this section facilitate explicit construction of the Markov matrix, and are necessary for proving correctness of the worm algorithm.

The key points about the structure of the fibration, formalized by the lemmas below, are:

- Each open permutation is one opener move away from a base closed permutation. The N open permutations above a base closed permutation π are the fiber over π.
- This induces a disjoint partition of the open permutations $\mathcal{S}_{N+1} \setminus \mathcal{S}_N$.
- Opens and closes stay within fibers; non-trivial head swaps and tail swaps cross fibers.
- For each open permutation, the six non-trivial head swaps and six tail swaps result in twelve distinct permutations.
- Head swaps and tail swaps are transitive on fibers.

We first define maps corresponding to worm Metropolis moves.

Definition 3.7.1. The four worm Metropolis moves of figure 4 may be viewed in terms of maps. Throughout, $\mathbf{z} \in \mathcal{L} \cup \{w\}$.

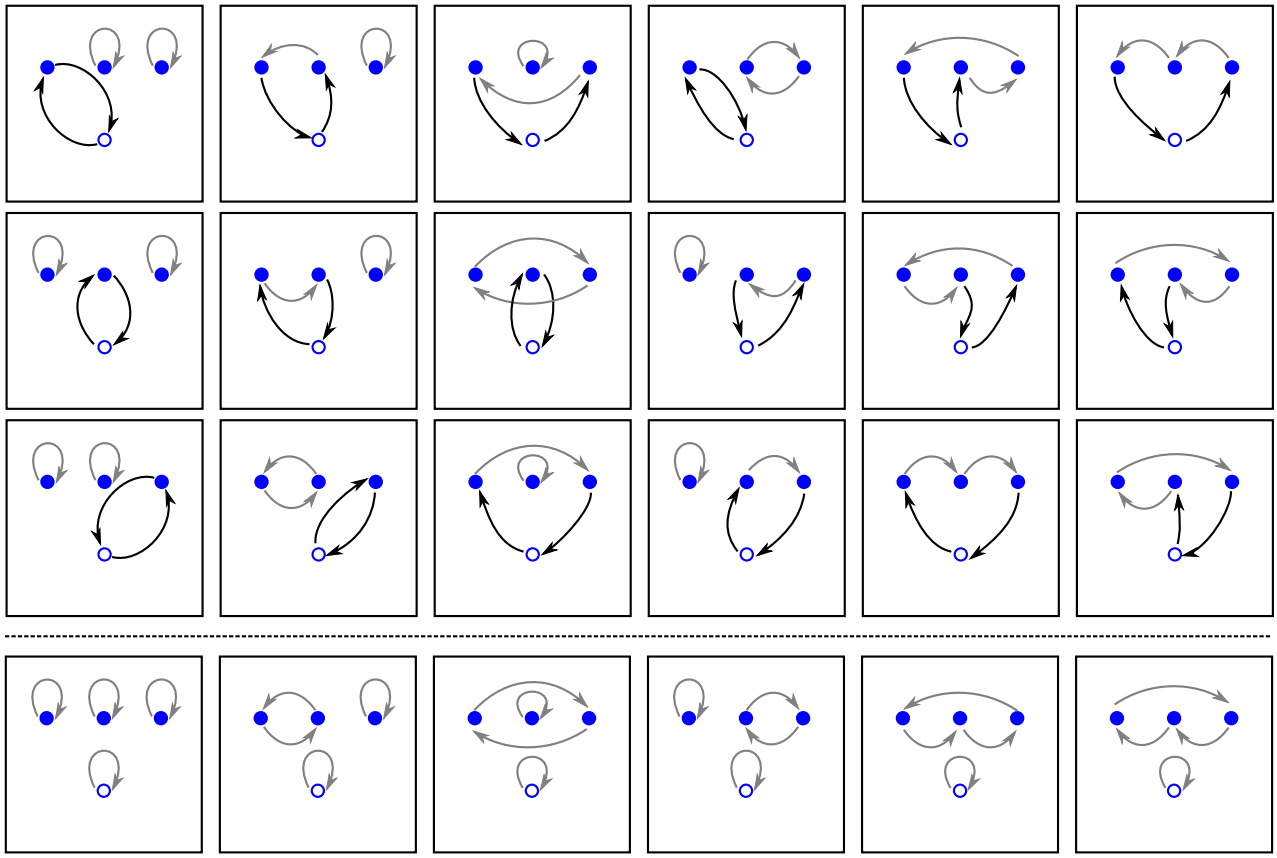

Figure 5: Fibration of $\mathcal{S}_4$ over $\mathcal{S}_3$. Closed permutations (i.e. $\mathcal{S}_3$) are along the bottom row; open permutations (i.e. $\mathcal{S}_4 \setminus \mathcal{S}_3$) are above the bottom row. The column, or fiber, above each closed permutation π contains the open permutations obtained from π by an opener move. Arrows modified by opener moves are shown in black.

Let $O: \mathcal{S}_N \times \mathcal{L} \to \mathcal{S}_{N+1} \setminus \mathcal{S}_N$ send $O(\pi, \mathbf{x}) = \pi'$ such that

$$\begin{aligned} \pi'(\mathbf{x}) &= w, \\ \pi'(w) &= \pi(\mathbf{x}), \\ \pi'(\mathbf{z}) &= \pi(\mathbf{z}), \quad \mathbf{z} \neq \mathbf{x}, w. \end{aligned}$$

Let $C: \mathcal{S}_{N+1} \setminus \mathcal{S}_N \to \mathcal{S}_N$ send $C(\pi) = \pi'$ such that

$$\begin{aligned} \pi'(\pi^{-1}(w)) &= \pi(w), \\ \pi'(w) &= w, \\ \pi'(\mathbf{z}) &= \pi(\mathbf{z}), \quad \mathbf{z} \neq \pi^{-1}(w), w. \end{aligned}$$

Let $S: \mathcal{S}_{N+1} \setminus \mathcal{S}_N \times \mathcal{L} \to \mathcal{S}_{N+1} \setminus \mathcal{S}_N$ send $S(\pi, \mathbf{x}) = \pi'$ such that

$$\begin{aligned} \pi'(\mathbf{x}) &= w, \\ \pi'(\pi^{-1}(w)) &= \pi(\mathbf{x}), \\ \pi'(\mathbf{z}) &= \pi(\mathbf{z}), \quad \mathbf{z} \neq \mathbf{x}, \pi^{-1}(w). \end{aligned}$$

Let $T:\ \mathcal{S}_{N+1} \setminus \mathcal{S}_N \times \mathcal{L} \to \mathcal{S}_{N+1} \setminus \mathcal{S}_N$ send $T(\pi, \mathbf{x}) = \pi'$ such that

$$\begin{aligned} \pi'(\mathbf{x}) &= \pi(w), \\ \pi'(w) &= \pi(\mathbf{x}), \\ \pi'(\mathbf{z}) &= \pi(\mathbf{z}), \quad \mathbf{z} \neq \mathbf{x}, w. \end{aligned}$$

Throughout the proofs of the fibration-structure lemmas, we will use the following fact.

Lemma 3.7.2. *If $\mathbf{x} \neq \mathbf{y}$, then $\pi(\mathbf{x}) \neq \pi(\mathbf{y})$ and $\pi^{-1}(\mathbf{x}) \neq \pi^{-1}(\mathbf{y})$.*

Proof. If $\mathbf{x} \neq \mathbf{y}$ and $\pi(\mathbf{x}) = \pi(\mathbf{y})$, then π is not 1-1 which is a contradiction since π is a permutation. This applies to π^{-1} as well, since π^{-1} is also a permutation. □

Now we may prove the fibration-structure lemmas.

Lemma 3.7.3. *Each open permutation π is one opener move away from a base closed permuation π'. That is, for all $\pi \in \mathcal{S}_{N+1} \setminus \mathcal{S}_N$, there exists $\pi' \in \mathcal{S}_N$ such that $C(\pi) = \pi'$.*

Proof. Let $\pi \in \mathcal{S}_{N+1}$. Since π is open, $\pi(w) \neq w$ and $\pi^{-1}(w) \neq w$. Let $\mathbf{a} = \pi^{-1}(w)$ and $\mathbf{b} = \pi(w)$. Both are lattice points. Applying C, we have $C(\pi) = \pi'$ where $\pi'(\mathbf{a}) = \mathbf{b}$, $\pi'(w) = w$, and $\pi'(\mathbf{z}) = \pi(\mathbf{z})$ for all remaining lattice points $\mathbf{z} \neq \mathbf{a}, \mathbf{b}$. Since $\pi'(w) = w$, π' is closed. □

Definition 3.7.4. For $\pi \in \mathcal{S}_N$, $C^{-1}(\pi) \subset \mathcal{S}_{N+1} \setminus \mathcal{S}_N$ is the **fiber** of open permutations over π.

Lemma 3.7.5. *Opens and closes stay within fibers, and each fiber has N elements.*

Proof. Closes stay within fibers by definition of fiber. Next, fix $\pi \in \mathcal{S}_N$ and let $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{L}$. (These are two different ways to open the same closed permutation.) Let

$$\pi'_1 = O(\pi, \mathbf{x}_1), \quad \pi'_2 = O(\pi, \mathbf{x}_2).$$

Then π'_1 and π'_2 have

$$\mathbf{x}_1 \mapsto w \mapsto \pi(\mathbf{x}_1), \qquad \mathbf{x}_2 \mapsto w \mapsto \pi(\mathbf{x}_2),$$

respectively, agreeing with π at all other lattice points $\mathbf{z}$. Now, $C(\pi'_1)$ and $C(\pi'_2)$ have

$$\mathbf{x}_1 \mapsto \pi(\mathbf{x}_1), w \mapsto w, \qquad \mathbf{x}_2 \mapsto \pi(\mathbf{x}_2), w \mapsto w$$

respectively, agreeing with π at all other lattice points $\mathbf{z}$. But this means $C(\pi'_1)$ agrees with $C(\pi'_2)$ agree at all points of $\mathcal{L}'$, so $C(\pi'_1) = C(\pi'_2)$. Thus, π'_1 and π'_2 are in the same fiber.

For the last claim, fix $\pi \in \mathcal{S}_N$ and enumerate the N lattice points of $\mathcal{L}$ as $\mathbf{x}_1, \ldots, \mathbf{x}_N$. We claim that the N permutations

$$\pi'_1 = O(\pi, \mathbf{x}_1), \ldots, \pi'_N = O(\pi, \mathbf{x}_N),$$

which are all now known to be in the same fiber, are all distinct. To see this, fix $i \neq j$ from out of $\{1, 2, \ldots, N\}$. Then π'_i and π'_j have

$$\mathbf{x}_i \mapsto w \mapsto \pi(\mathbf{x}_i), \qquad \mathbf{x}_j \mapsto w \mapsto \pi(\mathbf{x}_j).$$

Since $\mathbf{x}_i \neq \mathbf{x}_j$, by lemma 3.7.2 $\pi(\mathbf{x}_i) \neq \pi(\mathbf{x}_j)$. Since

$$\pi'_i(w) = \pi(\mathbf{x}_i) \neq \pi(\mathbf{x}_j) = \pi'_j(w),$$

π'_i and π'_j send w to different points. Therefore, the permutations π'_i and π'_j are distinct. □

Lemma 3.7.6. *This fibration induces a disjoint partition of the open permutations $\mathcal{S}_{N+1} \setminus \mathcal{S}_N$. That is, for $\pi_1', \pi_2' \in \mathcal{S}_N$,*

$$\pi_1' \neq \pi_2' \implies C^{-1}(\pi_1') \cap C^{-1}(\pi_2') = \emptyset \qquad \textit{and} \qquad \bigcup_{\pi \in \mathcal{S}_N} C^{-1}(\pi) = \mathcal{S}_{N+1} \setminus \mathcal{S}_N.$$

Proof. For the first claim, suppose the intersection is non-empty. Let $\pi \in \mathcal{S}_{N+1} \setminus \mathcal{S}_N$ be such that $\pi \in C^{-1}(\pi_1')$ and $\pi \in C^{-1}(\pi_2')$. This means $C(\pi) = \pi_1'$ and $C(\pi) = \pi_2'$ with $\pi_1' \neq \pi_2'$, which is a contradiction since the map C is uniquely defined for all $\pi \in \mathcal{S}_{N+1} \setminus \mathcal{S}_N$.

For the second claim: there are $N!$ closed permutations. We know from the first claim that the $N!$ fibers, one above each closed permutation, are all disjoint. From lemma 3.7.5, we know that each fiber has N elements. We have accounted for all $N \cdot N! = (N+1)! - N!$ open permutations, so we must have all of $\mathcal{S}_{N+1} \setminus \mathcal{S}_N$. □

Lemma 3.7.7. *Non-trivial head swaps and tail swaps (definition 3.6.1) cross fibers.*

Proof. First consider head swaps. Let $\pi, \pi' \in \mathcal{S}_{N+1} \setminus \mathcal{S}_N$ differ by a non-trivial head swap, namely, there is $\mathbf{x} \neq \pi^{-1}(w)$ such that $\pi' = S(\pi, \mathbf{x})$. Then π and π' have

$$\begin{array}{lccccccccccc} \pi: & & \mathbf{x} & \mapsto & \pi(\mathbf{x}) & \mapsto & \pi^2(\mathbf{x}), & & \pi^{-1}(w) & \mapsto & w & \mapsto & \pi(w), \\ \pi': & \pi^{-1}(w) & \mapsto & \pi(\mathbf{x}) & \mapsto & \pi^2(\mathbf{x}), & & & \mathbf{x} & \mapsto & w & \mapsto & \pi(w), \end{array}$$

respectively. Now apply C to each: $C(\pi)$ and $C(\pi')$ have

$$\begin{array}{lccccccccccc} C(\pi): & & \mathbf{x} & \mapsto & \pi(\mathbf{x}) & \mapsto & \pi^2(\mathbf{x}), & & \pi^{-1}(w) & \mapsto & \pi(w), & & w & \mapsto & w, \\ C(\pi'): & \pi^{-1}(w) & \mapsto & \pi(\mathbf{x}) & \mapsto & \pi^2(\mathbf{x}), & & & \mathbf{x} & \mapsto & \pi(w), & & w & \mapsto & w, \end{array}$$

respectively. Since $\mathbf{x} \neq \pi^{-1}(w)$, $C(\pi) \neq C(\pi')$.

Next, consider tail swaps. Let $\pi, \pi' \in \mathcal{S}_{N+1} \setminus \mathcal{S}_N$ differ by a non-trivial tail swap, namely, there is $\pi(\mathbf{x}) \neq \pi(w)$ such that $\pi' = T(\pi, \mathbf{x})$. Then π and π' have

$$\begin{array}{lccccccccccc} \pi: & \pi^{-1}(\mathbf{x}) & \mapsto & \mathbf{x} & \mapsto & \pi(\mathbf{x}), & & \pi^{-1}(w) & \mapsto & w & \mapsto & \pi(w), \\ \pi': & \pi^{-1}(\mathbf{x}) & \mapsto & \mathbf{x} & \mapsto & \pi(w), & & \pi^{-1}(w) & \mapsto & w & \mapsto & \pi(\mathbf{x}), \end{array}$$

respectively. Now apply C to each: $C(\pi)$ and $C(\pi')$ have

$$\begin{array}{lccccccccccc} C(\pi): & \pi^{-1}(\mathbf{x}) & \mapsto & \mathbf{x} & \mapsto & \pi(\mathbf{x}), & & \pi^{-1}(w) & \mapsto & \pi(w), & & w & \mapsto & w, \\ C(\pi'): & \pi^{-1}(w) & \mapsto & \mathbf{x} & \mapsto & \pi(w), & & \pi^{-1}(w) & \mapsto & \pi(\mathbf{x}), & & w & \mapsto & w, \end{array}$$

respectively. Since $\pi(\mathbf{x}) \neq \pi(w)$, $C(\pi) \neq C(\pi')$. □

Lemma 3.7.8. *For each open permutation, the six non-trivial head swaps and six non-trivial tail swaps result in twelve distinct permutations.*

Proof. Fix $\pi \in \mathcal{S}_{N+1} \setminus \mathcal{S}_N$. Let $\mathbf{x}_1, \ldots, \mathbf{x}_6$ be the six nearest-neighbor lattice sites to the lattice site $\pi^{-1}(w)$; let $\mathbf{y}_1, \ldots, \mathbf{y}_6$ be the six lattice sites such that $\pi(\mathbf{y}_1), \ldots, \pi(\mathbf{y}_6)$ are nearest-neighbor lattices site to the lattice site $\pi(w)$. (See figure 4.)

First, we show that the six permutations $S(\pi, \mathbf{x}_1), \ldots, S(\pi, \mathbf{x}_6)$ are distinct. Let $i \neq j$ for $i, j = 1, \ldots, 6$; let $\pi_i = S(\pi, \mathbf{x}_i)$ and $\pi_j = S(\pi, \mathbf{x}_j)$. Then π has

$$\pi: \quad \mathbf{x}_i \mapsto \pi(\mathbf{x}_i), \qquad \mathbf{x}_j \mapsto \pi(\mathbf{x}_j), \qquad \pi^{-1}(w) \mapsto w;$$

π_i, and π_j have

$$\begin{array}{lllll} \pi_i: & \mathbf{x}_i & \mapsto & w, & \pi^{-1}(w) \mapsto \pi(\mathbf{x}_i), \\ \pi_j: & \mathbf{x}_j & \mapsto & w, & \pi^{-1}(w) \mapsto \pi(\mathbf{x}_j), \end{array}$$

respectively. Since $\mathbf{x}_i \neq \mathbf{x}_j$, $\pi_i \neq \pi_j$.

Second, we show that the six permutations $T(\pi, \mathbf{y}_1), \ldots, T(\pi, \mathbf{y}_6)$ are distinct. Let $i \neq j$ for $i, j = 1, \ldots, 6$; let $\pi_i = T(\pi, \mathbf{y}_i)$ and $\pi_j = T(\pi, \mathbf{y}_j)$. Then π has

$$\pi: \quad \mathbf{y}_i \mapsto \pi(\mathbf{y}_i), \qquad \mathbf{y}_j \mapsto \pi(\mathbf{y}_j), \qquad w \mapsto \pi(w);$$

π_i, and π_j have

$$\begin{array}{lllll} \pi_i: & \mathbf{y}_i & \mapsto & \pi(w), & w \mapsto \pi(\mathbf{y}_i), \\ \pi_j: & \mathbf{y}_j & \mapsto & \pi(w), & w \mapsto \pi(\mathbf{y}_j), \end{array}$$

respectively. Since $\mathbf{y}_i \neq \mathbf{y}_j$, by lemma 3.7.2 $\pi(\mathbf{y}_i) \neq \pi(\mathbf{y}_j)$. Since π_i, π_j send w to to different sites, $\pi_i \neq \pi_j$.

Third, we show that the head-swaps of π are distinct from the tail-swaps of π. Fix $\pi \in \mathcal{S}_{N+1} \setminus \mathcal{S}_N$ and let $i, j \in \{1, \ldots, 6\}$. Then π has

$$\pi: \quad \mathbf{x}_i \mapsto \pi(\mathbf{x}_i), \qquad \mathbf{y}_j \mapsto \pi(\mathbf{y}_j), \qquad \pi^{-1}(w) \mapsto w \mapsto \pi(w);$$

$S(\pi, \mathbf{x}_i)$ and $T(\pi, \mathbf{y}_j)$ have

$$\begin{array}{lllll} S(\pi, \mathbf{x}_i): & \pi^{-1}(w) & \mapsto & \pi(\mathbf{x}_i), & \mathbf{x}_i \mapsto w \mapsto \pi(w); \\ T(\pi, \mathbf{y}_j): & \mathbf{y}_j & \mapsto & \pi(w), & \pi^{-1}(w) \mapsto w \mapsto \mathbf{y}_j; \end{array}$$

respectively. Under these two permutations, w has images $\pi(w)$ and $\mathbf{y}_j$, respectively, and preimages $\mathbf{x}_i$ and $\pi^{-1}(w)$. By definition 3.6.1, the non-trivial head swap $S(\pi, \mathbf{x}_i)$ has $\mathbf{x}_i \neq \pi^{-1}(w)$ and the non-trivial tail swap $T(\pi, \mathbf{y}_j)$ has $\pi(w) \neq \mathbf{y}_j$. Thus, $S(\pi, \mathbf{x}_i)$ and $T(\pi, \mathbf{y}_j)$ are distinct permutations. □

Lemma 3.7.9. *Head swaps and tail swaps are transitive on fibers.*

Proof. This needs to be proved. This key result will establish irreducibility of the chain. □

3.8 Explicit construction of the Markov matrix

Transition probabilities were described as being proportional to $1 \wedge e^{-\Delta H}$. We put the constants of proportionality to be:

- a for head swaps and tail swaps;
- b for closer moves;
- c for opener moves.

For GRU, we chose C solely by the row-normalization condition. Here, with a more complicated algorithm, we will choose them to satisfy detailed balance.

The Markov matrix is now $(N+1)! \times (N+1)!$:

- A closed permutation transitions only to itself, or to any of the N open permutations in the fiber above it. Thus, there are $N+1$ non-zero entries in π's row of $\mathbf{M}$.

- An open permutation transitions to any of the 12 open permutations available by head-swapping or tail-swapping, or to itself, or to the closed permutation at the base of its fiber. Thus, there are 14 non-zero entries in π's row of $\mathbf{M}$.

Definition 3.8.1. For open π, let

$$\{\mathbf{x}_1, \dots, \mathbf{x}_6\} = \{\mathbf{x} \in \mathcal{L} : \|\mathbf{x}, \pi^{-1}(w)\| = 1\} \qquad \text{and} \qquad \{\mathbf{y}_1, \dots, \mathbf{y}_6\} = \{\mathbf{y} \in \mathcal{L} : \|\pi(\mathbf{y}), \pi(w)\| = 1\}.$$

Then define

$$R_S(\pi) = \{S(\pi, \mathbf{x}_1), \dots, S(\pi, \mathbf{x}_6)\},$$
$$R_T(\pi) = \{T(\pi, \mathbf{y}_1), \dots, T(\pi, \mathbf{y}_6)\}.$$

These are the twelve open permutations reachable from π via head swaps and tail swaps, respectively (lemma 3.7.8). For closed π, define

$$R_O(\pi) = \{O(\pi, \mathbf{x}_1), \dots, O(\pi, \mathbf{x}_N)\}.$$

These are the N open permutations reachable from π via opener moves.

The entries of the transition matrix are as follows.

If π is closed:

$$M(\pi, \pi') = \begin{cases} c\left(1 \wedge e^{-H(\pi')+H(\pi)}\right), & \pi' \in R_O(\pi); \\ 1 - \displaystyle\sum_{\pi' \in R_O(\pi)} c\left(1 \wedge e^{-H(\pi')+H(\pi)}\right), & \pi' = \pi; \\ 0, & \text{otherwise.} \end{cases}$$

If π is open:

$$M(\pi, \pi') = \begin{cases} a\left(1 \wedge e^{-H(\pi')+H(\pi)}\right), & \pi' \in R_S(\pi); \\ a\left(1 \wedge e^{-H(\pi')+H(\pi)}\right), & \pi' \in R_T(\pi); \\ b\left(1 \wedge e^{-H(\pi')+H(\pi)}\right), & \pi' = C(\pi); \\ 1 - \displaystyle\sum_{\pi' \in R_S(\pi) \cup R_T(\pi)} a\left(1 \wedge e^{-H(\pi')+H(\pi)}\right) - b\left(1 \wedge e^{-H(C(\pi))+H(\pi)}\right), & \pi' = \pi; \\ 0, & \text{otherwise.} \end{cases}$$

Row normalization for closed π: $c(1 \wedge e^{-\Delta H})$ is between 0 and c so $\sum$rest is between 0 and cN. Take

$$c = 1/N. \tag{3.8.2}$$

Row normalization for open π:

$$12a + b \leq 1. \tag{3.8.3}$$

3.9 Correctness

Proposition 3.9.1 (Irreducibility)**.** *The worm algorithm's Markov chain is irreducible.*

Proof. As for the GRU algorithm, this non-trivial result needs to be proved. □

We mention some partial results.

Proposition 3.9.2. *The worm algorithm's Markov chain is irreducible if the GRU algorithm's Markov chain is irreducible.*

Proof. The key point is that the composition of an open, head swap, and close are precisely a GRU swap. Let $\mathbf{x}$ and $\mathbf{y}$ be lattice points such that $\pi(\mathbf{x})$ and $\pi(\mathbf{y})$ are nearest neighbors. Starting with π, then applying an open at $\mathbf{x}$, a head swap at $\mathbf{y}$, and a close, we have

$$\begin{array}{lccccccccc}
\pi: & \mathbf{x} & \mapsto & \pi(\mathbf{x}), & \mathbf{y} & \mapsto & \pi(\mathbf{y}), & w & \mapsto & w; \\
\pi' = O(\pi, \mathbf{x}): & \mathbf{x} & \mapsto & w, & \mathbf{y} & \mapsto & \pi(\mathbf{y}), & w & \mapsto & \pi(\mathbf{x}); \\
\pi'' = S(\pi', \mathbf{y}): & \mathbf{x} & \mapsto & \pi(\mathbf{y}), & \mathbf{y} & \mapsto & w, & w & \mapsto & \pi(\mathbf{x}); \\
\pi''' = C(\pi''): & \mathbf{x} & \mapsto & \pi(\mathbf{y}), & \mathbf{y} & \mapsto & \pi(\mathbf{x}), & w & \mapsto & w.
\end{array}$$

This shows that, if the GRU algorithm is irreducible on $\mathcal{S}_N$, the worm algorithm is irreducible on $\mathcal{S}_N$. But then the worm algorithm is also irreducible on $\mathcal{S}_{N+1}$: fix an initial and final permutation; close the initial permutation, if it is open, to obtain a closed permutation; use the preceding argument to reach the closed permutation which lies under the fiber of the desired final open permutation; do an open move (see lemma 3.7.5) if the final permutation is open. □

Remark 3.9.3. The worm algorithm has an addtional degree of freedom. If $\mathbf{x}$ and $\mathbf{y}$ are nearest-neighbor lattice sites, then the composition of an open at $\mathbf{x}$, a tail swap at $\mathbf{y}$, and a close results in a similar swap of the jump targets of $\mathbf{x}$ and $\mathbf{y}$:

$$\begin{array}{lccccccccc}
\pi: & \mathbf{x} & \mapsto & \pi(\mathbf{x}), & \mathbf{y} & \mapsto & \pi(\mathbf{y}), & w & \mapsto & w; \\
\pi' = O(\pi, \mathbf{x}): & \mathbf{x} & \mapsto & w, & \mathbf{y} & \mapsto & \pi(\mathbf{y}), & w & \mapsto & \pi(\mathbf{x}); \\
\pi'' = T(\pi', \mathbf{y}): & \mathbf{x} & \mapsto & w, & \mathbf{y} & \mapsto & \pi(\mathbf{x}) & w & \mapsto & \pi(\mathbf{y}); \\
\pi''' = C(\pi''): & \mathbf{x} & \mapsto & \pi(\mathbf{y}), & \mathbf{y} & \mapsto & \pi(\mathbf{x}), & w & \mapsto & w.
\end{array}$$

Proposition 3.9.4 (Aperiodicity)**.** *The worm algorithm's Markov chain is aperiodic.*

Proof. This is essentially the same as in the GRU algorithm (proposition 2.4.3): given the small positive γ in equation 3.4.3, an opener move from the identity entails an increase in energy, and thus a reject of such an opener move occurs with a non-zero probability.

(This argument applies in the non-interacting case. For N_2 and N_ℓ, it also applies. For V_{ij}, we need to check that an opener move from the identity doesn't decrease energy.) □

Proposition 3.9.5 (Detailed balance)**.** *The Markov chain of the worm algorithm satisfies detailed balance with $b = c$.*

Proof. We need

$$P'(\pi)M(\pi, \pi') = P'(\pi')M(\pi', \pi).$$

For closed π to closed π': If $\pi = \pi'$ then we have detailed balance trivially. If $\pi \neq \pi'$ then $M(\pi, \pi') = M(\pi', \pi) = 0$ since there are no transitions between distinct closed permutations.

For closed π to open π': If π' is not in the fiber above π, then $M(\pi,\pi') = M(\pi',\pi) = 0$ since opens and closes respect fibers (lemma 3.7.5). Now suppose π' is in the fiber above π. As in the GRU algorithm (proposition 2.4.4), do cases on ΔH positive or negative. If $H'(\pi') \le H'(\pi)$, then

$$e^{-H'(\pi)}c = e^{-H'(\pi')}be^{-H'(\pi)}e^{H'(\pi')}.$$

Choose

$$b = c \tag{3.9.6}$$

to satisfy detailed balance. The case $H'(\pi') > H'(\pi)$ results in the same $b = c$ condition.

For open π to closed π': If π is not in the fiber above π', then $M(\pi,\pi') = M(\pi',\pi) = 0$ (lemma 3.7.5). If π is in the fiber above π', then we recover the $b = c$ condition.

It now remains to consider open π transitioning to open π'. We assume this to be the case for the rest of the proof.

If $M(\pi,\pi') = 0$ then we claim $M(\pi',\pi) = 0$, as in lemma 2.4.6. We have $\pi' \neq \pi$, $\pi' \notin R_S(\pi)$, and $\pi' \notin R_T(\pi)$. We need to show $\pi \neq \pi'$ (which is obvious), $\pi \notin R_S(\pi')$, and $\pi \notin R_T(\pi')$. We prove the contrapositive:

$$\pi \in \{\pi'\} \cup R_S(\pi') \cup R_T(\pi') \quad \Longrightarrow \quad \pi' \in \{\pi\} \cup R_S(\pi) \cup R_T(\pi).$$

If $\pi = \pi'$ then detailed balance is trivially satisfied. Suppose $\pi \in R_S(\pi')$. Then for some $\mathbf{x}_i$, $i = 1,\dots,6$, π' and π have

$$\begin{array}{lccccccc} \pi': & \mathbf{x}_i & \mapsto & \pi'(\mathbf{x}_i), & \pi^{-1}(w) & \mapsto & w & \mapsto & w, \\ \pi: & \mathbf{x}_i & \mapsto & w, & \pi^{-1}(w) & \mapsto & w & \mapsto & \pi'(\mathbf{x}_i). \end{array}$$

The lattice sites $\mathbf{x}_i$ and w are nearest neighbors and π', π agree at all other sites, so there is a head swap sending π to π'. The case $\pi \in \mathbb{R}_T(\pi')$ is completely analogous. This completes the proof of the claim that $M(\pi,\pi') = 0 \implies M(\pi',\pi) = 0$.

If $M(\pi,\pi') \neq 0$ then we claim $M(\pi',\pi) \neq 0$, again as in lemma 2.4.6. The logic is the same as in the contrapositive argument which was just completed.

The last step is to show detailed balance for open π, π' where $M(\pi,\pi') \neq 0$. Again we do cases on whether the energy decreases or increases. If $H'(\pi') \le H'(\pi)$, then equation 3.9.6 is

$$ae^{-H'(\pi)}(1) = ae^{-H'(\pi')}\left(e^{-H'(\pi)}e^{H'(\pi')}\right).$$

If $H'(\pi') > H'(\pi)$, then we have

$$ae^{-H'(\pi)}\left(e^{-H'(\pi')}e^{H'(\pi)}\right) = ae^{-H'(\pi')}(1).$$

In either case, detailed balance holds. □

Remark. Note that for closed π, there are N choices of open π'; for open π, there is one choice of closed π'. In the software implementation, the $1/N$ for opens comes in through uniform-random choice of $\mathbf{x} \in \mathcal{L}$. The result is that, for closed π, one may only attempt an open. For open π, one attempts a close $1/N$ of the time, and head or tail swaps each half the rest of the time, respectively.

As a sanity check, we point out that cycles may grow or shrink upon worm moves.

Proposition 3.9.7. *Non-trivial worm head swaps and tail swaps either split one cycle into two, or join two cycles into one.*

Proof. This is the same as for the GRU case (proposition 3.9.7), which is strictly an algebraic result: the non-spatiality of the w point plays no role. □

4 ΔH computations

When computing ΔH for the GRU or worm algorithms, it is inefficient to find $H(\pi')$ and $H(\pi)$ separately, then compute their difference: GRU and worm moves are local, and most of the energy terms are unchanged from π to π'. Instead (this is true for Metropolis simulations in general), one discovers a formula for the energy change in a proposed Metropolis move. Even though these minimal energy-change formulas are a software-optimization detail, they need to be considered carefully lest errors intrude.

4.1 GRU and worm with N_2 interactions

The non-spatiality of the wormhole point plays no role in the algebraic notion of cycle lengths. Thus, the same ΔN_2 formulas apply to both algorithms.

Recall the definition of GRU swap from section 2.2. The simplicity of figure 6 masks a bit of detail: namely, the four points may not all be distinct. Thus, there are several cases. (See figure 7.)

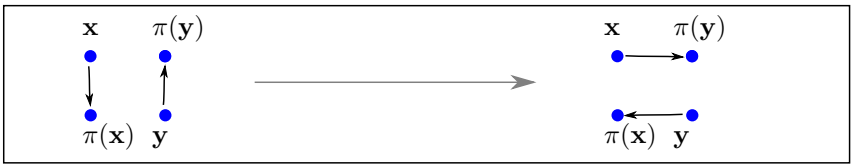

Figure 6: GRU swap.

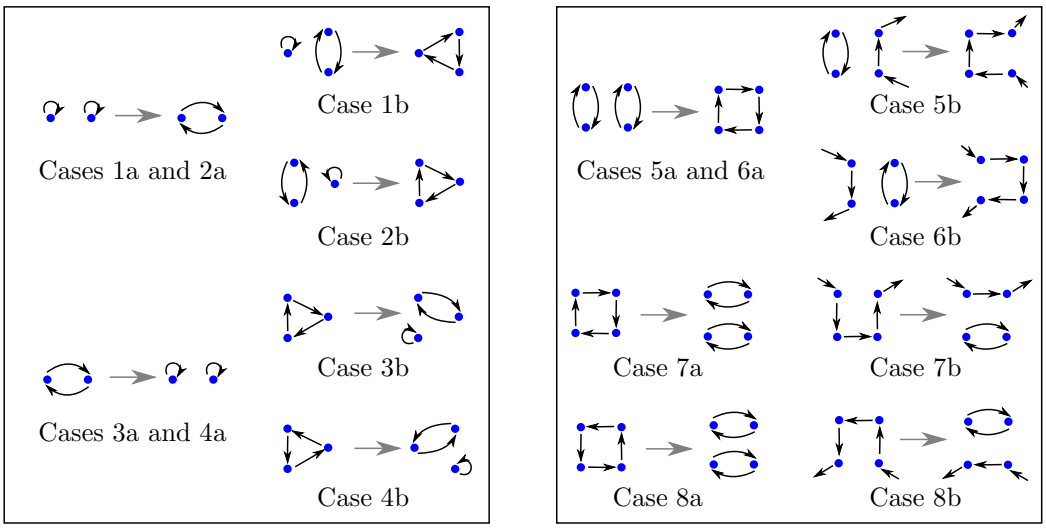

Figure 7: Cases for ΔN_2.

- Case 0: $\pi(\mathbf{x}) = \pi(\mathbf{y})$ (and so also $\mathbf{x} = \mathbf{y}$): this is a trivial GRU move; $\pi' = \pi$. $\Delta N_2 = 0$.
- Case 1: $\mathbf{x} = \pi(\mathbf{x})$.
  - Case 1a: $\mathbf{y} = \pi(\mathbf{y})$. $\Delta N_2 = +1$.

  - Case 1b: $\mathbf{y} \neq \pi(\mathbf{y})$ but $\mathbf{y} = \pi^2(\mathbf{y})$. $\Delta N_2 = -1$.
  - Case 1c: $\mathbf{y} \neq \pi(\mathbf{y}), \pi^2(\mathbf{y})$. $\Delta N_2 = 0$.
- Case 2: $\mathbf{y} = \pi(\mathbf{y})$.
  - Case 2a: $\mathbf{x} = \pi(\mathbf{x})$. Same as case 1a. $\Delta N_2 = +1$.
  - Case 2b: $\mathbf{x} \neq \pi(\mathbf{x})$ but $\mathbf{x} = \pi^2(\mathbf{x})$. $\Delta N_2 = -1$.
  - Case 2c: $\mathbf{x} \neq \pi(\mathbf{x}), \pi^2(\mathbf{x})$. $\Delta N_2 = 0$.
- Case 3: $\mathbf{x} = \pi(\mathbf{y})$.
  - Case 3a: $\pi(\mathbf{x}) = \mathbf{y}$. $\Delta N_2 = -1$.
  - Case 3b: $\pi^2(\mathbf{x}) = \mathbf{y}$. $\Delta N_2 = +1$.
  - Case 3c: $\mathbf{y} \neq \pi(\mathbf{x}), \pi^2(\mathbf{x})$. $\Delta N_2 = 0$.
- Case 4: $\pi(\mathbf{x}) = \mathbf{y}$.
  - Case 4a: $\pi(\mathbf{y}) = \mathbf{x}$. Same as case 3a. $\Delta N_2 = -1$.
  - Case 4b: $\pi^2(\mathbf{y}) = \mathbf{x}$. $\Delta N_2 = +1$.
  - Case 4c: $\mathbf{x} \neq \pi(\mathbf{y}), \pi^2(\mathbf{y})$. $\Delta N_2 = 0$.
- Case 5: $\pi^2(\mathbf{x}) = \mathbf{x}$.
  - Case 5a: $\pi^2(\mathbf{y}) = \mathbf{y}$. $\Delta N_2 = -2$.
  - Case 5b: $\pi^2(\mathbf{y}) \neq \mathbf{y}$. $\Delta N_2 = -1$.
- Case 6: $\pi^2(\mathbf{y}) = \mathbf{y}$.
  - Case 6a: $\pi^2(\mathbf{x}) = \mathbf{x}$. Same as 5a. $\Delta N_2 = -2$.
  - Case 6b: $\pi^2(\mathbf{x}) \neq \mathbf{x}$. $\Delta N_2 = -1$.
- Case 7: $\pi^2(\mathbf{x}) = \mathbf{y}$.
  - Case 7a: $\pi^2(\mathbf{y}) = \mathbf{x}$. $\Delta N_2 = +2$.
  - Case 7b: $\pi^2(\mathbf{y}) \neq \mathbf{x}$. $\Delta N_2 = +1$.
- Case 8: $\pi^2(\mathbf{y}) = \mathbf{x}$.
  - Case 8a: $\pi^2(\mathbf{x}) = \mathbf{y}$. $\Delta N_2 = +2$.
  - Case 8b: $\pi^2(\mathbf{x}) \neq \mathbf{y}$. $\Delta N_2 = +1$.
- All other cases: $\Delta N_2 = 0$.

4.2 GRU and worm with N_ℓ interactions

The non-spatiality of the wormhole point plays no role in the algebraic notion of cycle lengths. Thus, the same ΔN_2 formulas apply to both algorithms.

Recall proposition 2.4.7: if $\mathbf{x}$ and $\mathbf{y}$ are in separate cycles before the swap, they are in the same cycle afterward, and vice versa. Throughout this section, please consult figure 8 for illumination.

- Case 0: $\pi(\mathbf{x}) = \pi(\mathbf{y})$ (and so also $\mathbf{x} = \mathbf{y}$): this is a trivial GRU move; $\pi' = \pi$. $\Delta N_2 = 0$.

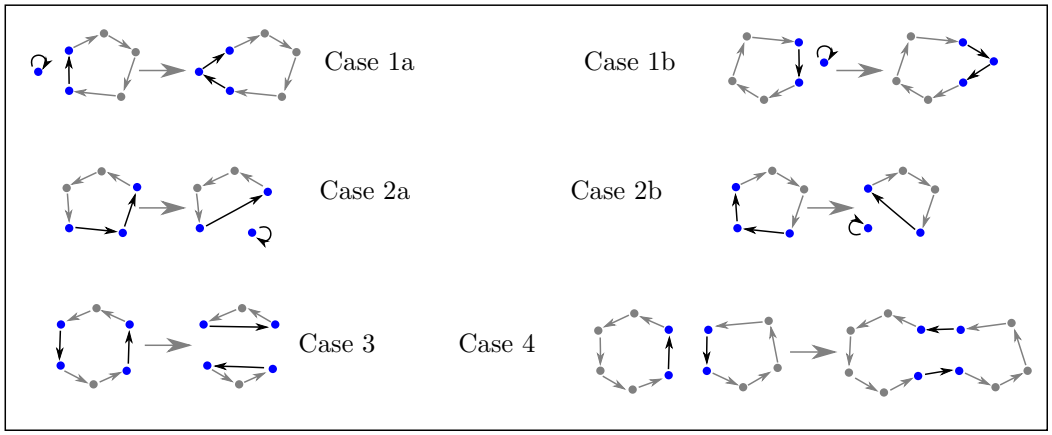

Figure 8: Cases for ΔN_ℓ. Sites and arrows not participating in changes are shown in grey.

- Case 1: $\mathbf{x}$ and $\mathbf{y}$ are in different cycles, but one of them is in a one-cycle.
  - Case 1a: $\mathbf{x} = \pi(\mathbf{x})$: $\Delta N_1 = -1$, $\Delta N_{\ell_\pi(\mathbf{y})} = -1$, $\Delta N_{\ell_\pi(\mathbf{y})+1} = +1$.
  - Case 1b: $\mathbf{y} = \pi(\mathbf{y})$: $\Delta N_1 = -1$, $\Delta N_{\ell_\pi(\mathbf{x})} = -1$, $\Delta N_{\ell_\pi(\mathbf{x})+1} = +1$.
- Case 2: $\mathbf{x}$ and $\mathbf{y}$ are in the same cycle, but one is the jump target of the other.
  - Case 2a: $\mathbf{y} = \pi(\mathbf{x})$. $\Delta N_{\ell_\pi(\mathbf{x})} = -1$, $\Delta N_{\ell_\pi(\mathbf{x})-1} = +1$, $\Delta N_1 = +1$.
  - Case 2a: $\mathbf{x} = \pi(\mathbf{y})$. $\Delta N_{\ell_\pi(\mathbf{y})} = -1$, $\Delta N_{\ell_\pi(\mathbf{y})-1} = +1$, $\Delta N_1 = +1$.
- Case 3: $\mathbf{x}$ and $\mathbf{y}$ are in the same cycle, and neither is the jump target of the other. Let a be the smallest positive integer such that $\pi^a(\mathbf{x}) = \mathbf{y}$; let b be the smallest positive integer such that $\pi^b(\mathbf{x}) = \mathbf{x}$. $\Delta N_{a+b} = -1$, $\Delta N_a = +1$, $\Delta N_b = +1$.
- Case 4: $\mathbf{x}$ and $\mathbf{y}$ are in separate cycles. $\Delta N_{\ell_\pi(\mathbf{x})} = -1$, $\Delta N_{\ell_\pi(\mathbf{y})} = -1$, $\Delta N_{\ell_\pi(\mathbf{x})+\ell_\pi(\mathbf{y})} = +1$.

4.3 GRU with V interactions

Recall from proposition 3.5.1 that as long as the extended energy function H' agrees with the energy function H on closed cycles, P' has the correct marginal distribution on closed cycles. Thus, when writing energy terms for open cycles, we can choose how to define the energy. For N_2 and N_ℓ (the previous two sections), it is simplest to say that the non-spatial point w can partcipate in permutation cycles. For other interactions that depend on the spatiality of points, it is simplest to say that w does not participate. Thus, here we split out GRU and worm cases.

The change in energy is simply the contributions from the old arrows $\mathbf{x} \mapsto \pi(\mathbf{x})$ and $\mathbf{y} \mapsto \pi(\mathbf{y})$ to all other arrows, along with their mutual interaction, subtracted from the contributions from the new arrows $\mathbf{x} \mapsto \pi(\mathbf{y})$ and $\mathbf{y} \mapsto \pi(\mathbf{x})$ to all other arrows, along with their mutual interaction.

$$\sum_{\mathbf{v}\neq\mathbf{x},\mathbf{y}} V(\mathbf{x},\pi(\mathbf{y}),\mathbf{v},\pi(\mathbf{v})) + \sum_{\mathbf{v}\neq\mathbf{x},\mathbf{y}} V(\mathbf{y},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})) + V(\mathbf{x},\pi(\mathbf{y}),\mathbf{y},\pi(\mathbf{x}))$$
$$- \sum_{\mathbf{v}\neq\mathbf{x},\mathbf{y}} V(\mathbf{x},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})) - \sum_{\mathbf{v}\neq\mathbf{x},\mathbf{y}} V(\mathbf{y},\pi(\mathbf{y}),\mathbf{v},\pi(\mathbf{v})) - V(\mathbf{x},\pi(\mathbf{x}),\mathbf{y},\pi(\mathbf{y})).$$

4.4 Worm with V interactions

The non-spatial point has no interactions, so we simply track the creation and destruction of spatial-to-spatial arrows for the four types of worm move.

Open:

$$- \sum_{\mathbf{v}\neq\mathbf{x},w} V(\mathbf{x},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})).$$

Close:

$$\sum_{\mathbf{v}\neq\pi^{-1}(w),w} V(\pi^{-1}(w),\pi(w),\mathbf{v},\pi(\mathbf{v})).$$

Head swap:

$$\sum_{\mathbf{v}\neq\mathbf{x},\pi^{-1}(w)} V(\pi^{-1}(w),\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})) - \sum_{\mathbf{v}\neq\mathbf{x},\pi^{-1}(w)} V(\mathbf{x},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})).$$

Tail swap:

$$\sum_{\mathbf{v}\neq\mathbf{x},w} V(\mathbf{x},\pi(w),\mathbf{v},\pi(\mathbf{v})) - \sum_{\mathbf{v}\neq\mathbf{x},w} V(\mathbf{x},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})).$$

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