Snapshot Observation for 2D Classical Lattice Models
by Corner Transfer Matrix Renormalization Group

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We report a way of obtaining a spin configuration snapshot, which is one of the representative spin configurations in canonical ensemble, in a finite area of infinite size two-dimensional (2D) classical lattice models. The corner transfer matrix renormalization group (CTMRG), a variant of the density matrix renormalization group (DMRG), is used for the numerical calculation. The matrix product structure of the variational state in CTMRG makes it possible to stochastically fix spins each by each according to the conditional probability with respect to its environment.

§1. Introduction

For a classical lattice spin system that interacts with a reservoir, the spin configuration observed at an instant, which we call snapshot in the following, is one of the representative configurations in the canonical ensemble. Such a snapshot is experimentally observed if the time scale of the observation is much shorter than that of the evolution of the system. A frozen spin configuration after sudden cooling can also be regarded as a kind of snapshot. In general, snapshots show rough outlook of the system. For example, the typical size of a spin inverted island in the ordered state is of the order of the correlation length, and symmetries of ordered states can be intuitively identified. Figure 1 shows a snapshot inside the area of 100 by 100 of the two-dimensional (2D) ferromagnetic Ising model, where the system size is much larger than the shown region. Normally such a snapshot is drawn by Monte Carlo simulation,1) while the shown one is created by the corner transfer matrix renormalization group 2) (CTMRG), a variant of the density matrix renormalization group 2) (DMRG) applied to 2D classical lattice models. So far both DMRG and CTMRG have been used for calculations of thermal average of spin correlation functions, but not for the snapshots.

In this article we report a way of obtaining the conditional probability for a row of spins of length \(N\) surrounded by the rest of the system, using the matrix product structure 3) (MPS) of the variational state employed in CTMRG and DMRG. These spins can be fixed one by one according to the conditional probability, and after fixing all the spins in the row it is possible to obtain the conditional probability for the next row in the same manner. Applying such a fixing process for \(M\) numbers of rows, one obtains a snapshot for the area of \(N\) by \(M\) in infinite — or sufficiently large — 2D lattice systems. Numerical cost for this snapshot observation is of the same order of conventional zipping process in the finite system DMRG algorithm 2, 4.

In the next section we briefly explain how to fix a spin in the 2D lattice model in terms of the corner transfer matrix formalism. In section 3 we generalize the spin fixing procedure to a row of spins of the length \(N\), by taking partial sum for the inner product between MPSs. Introducing position dependence to the local factors that construct MPS, we successively fix the \(M\)-rows of spins as we explain in Sec.4. In the last section we conclude the result and discuss the relation with quantum observation in one dimension.

§2. One Spin Fixing

The corner transfer matrix (CTM), which was invented by Baxter,5) is not only useful for rigorous analyses of 2D lattice systems, but also efficient for numerical calculations of thermodynamic functions, especially away from the critical point. Let us briefly look at the construction of CTM and the block spin transformation applied for it.

We consider the square lattice Ising model as an example of the 2D classical lattice spin models. The partition function of the system is expressed as

\[
Z = \sum_{\{\sigma\}} \exp(H\{\sigma\}),
\]

(2.1)
where \( \{ \sigma \} \) represents a configuration of Ising spins \( \sigma = \pm 1 \) on the square lattice, and \( H(\sigma) \) is the Ising Hamiltonian, that is a sum of Ising interaction over all the bonds.

In the CTM formalism, the 2D lattice is divided into 4 parts, so called the quadrants or the corners.\(^5\) Let us label each quadrant as \( A, B, C, \) and \( D \). The Hamiltonian \( H(\sigma) \) is then expressed as sum of the corresponding parts

\[
H_A(\sigma_A) + H_B(\sigma_B) + H_C(\sigma_C) + H_D(\sigma_D),
\]

(2.2)

where \( \{ \sigma_A \}, \{ \sigma_B \}, \{ \sigma_C \}, \) and \( \{ \sigma_D \} \) denote spin configurations in each quadrant of the system. Note that neighboring quadrants share the same spins at the boundary between them. In this way the Boltzmann weight of the whole system is expressed as a product of 4 factors

\[
\exp(H(\sigma)) = \exp(H_A(\sigma_A)) \exp(H_B(\sigma_B)) \exp(H_C(\sigma_C)) \exp(H_D(\sigma_D)).
\]

(2.3)

The corner transfer matrix is the partial sum of each factor with respect to the spins inside the corner

\[
A(\alpha \sigma \beta) = \sum_{\{ \sigma_A \}} \exp(H_A(\sigma_A))
\]

(2.4)

except for those spins at the boundary with other corners, where the notation \( \sum' \) denotes this restricted summation, and where \( \alpha \) and \( \beta \) denotes groups of spins at the boundary. (See Fig. 2 (a).) The CTM is a block diagonal matrix with respect to \( \sigma \), while in this article we do not use this matrix property explicitly. Other CTMs \( B, C, \) and \( D \) are defined in the same manner. If the system is invariant under the rotation of 90 degree these CTMs are equivalent. For simplicity, we assume this symmetry in the following.

The matrix dimension of the CTM increases exponentially with the system size. In order to avoid this blow up and treat the CTM accurately in numerical calculation, block spin transformation is introduced in CTM RG from those spins \( \alpha \) and \( \beta \) at the boundary to \( m \)-state auxiliary variables. Such a transformation maps the CTM \( A \) into the compressed (or renormalized) one

\[
A(\xi \sigma \nu) = \sum_{\alpha \beta} U_\xi(\alpha) U_\nu(\beta) A(\alpha \sigma \beta),
\]

(2.5)

where \( \xi \) and \( \nu \) are the \( m \)-state auxiliary variables. The transformation matrix \( U_\xi(\alpha) \) is obtained by diagonalizing the density matrix \( \rho = ABCD.\(^2,6\) \) Other CTMs can also be mapped to \( B(\nu \sigma \eta), C(\eta \sigma \mu), \) and \( D(\mu \sigma \xi) \) as shown in Fig. 2 (b). The approximate partition function

\[
Z' = \sum_{\xi \sigma \nu \eta} A(\xi \sigma \nu) B(\nu \sigma \eta) C(\eta \sigma \mu) D(\mu \sigma \xi)
\]

(2.6)

is close enough to the original one \( Z \) in Eq. (2.1) if \( m \) is sufficiently large; normally \( m \) is of the order of 10 to 1000.

When the system size is far larger than the correlation length of the system, the renormalized CTMs becomes independent of the system size except for a constant multiple. Throughout this article we assume such a condition, and regard the renormalized CTM as a quadrant of infinite size systems.

Now we calculate the probability of observing \( \sigma = 1 \) (up) and \( \sigma = -1 \) (down) at the center of the system. We first prepare two partial sums

\[
L(\eta \sigma \xi) = \sum_{\mu} C(\eta \sigma \mu) D(\mu \sigma \xi)
\]

\[
R(\xi \sigma \eta) = \sum_{\nu} A(\xi \sigma \nu) B(\nu \sigma \eta),
\]

(2.7)

that we regard \( 2m^2 \)-dimensional vectors in the following. Figure 3 shows the graphical representation of the above equation. The order of variables in \( L(\eta \sigma \xi) \) is opposite to that of \( R(\xi \sigma \eta) \), since we keep the order of auxiliary variables in the right hand sides of the above equations. The approximate partition function \( Z' \) is represented as

\[
Z' = \langle L|R \rangle \equiv \sum_{\xi \sigma \eta} L(\eta \sigma \xi) R(\xi \sigma \eta),
\]

(2.8)

where we have introduced bracket notations for the book keeping. The probability of \( \sigma \) taking the specific value \( \bar{\sigma} \) can be written as

\[
p(\bar{\sigma}) = \frac{\langle L|\delta(\bar{\sigma}, \sigma)|R \rangle}{\langle L|R \rangle} = \sum_{\xi \sigma \eta} L(\eta \sigma \xi) R(\xi \sigma \eta) \sum_{\xi \sigma \eta} L(\eta \sigma \xi) R(\xi \sigma \eta),
\]

(2.9)

where the probability satisfies the normalization \( p(1) + p(-1) = 1 \). Therefore, creating a random number \( x \) in the range \([0,1)\) one can fix \( \sigma \) to \( \bar{\sigma} = 1 \) if \( x < p(1) \), otherwise to \( \bar{\sigma} = -1 \).
§3. Snapshot in a row

Let us generalize the spin fixing procedure to a \(N\) numbers of spins in a row from \(\sigma_1\) to \(\sigma_N\), where \(N\) is much smaller than the system size. For this purpose we introduce the half-row transfer matrices (HRTMs), that are upper and lower halves of the transfer matrix \(T\) to the horizontal direction. Figure 4 shows the system that we consider in this section. Between the vectors \(L\) and \(R\), there are \(N - 1\) numbers of transfer matrix

\[ T_i = S_i P_i \]  
(3.1)

from \(i = 1\) to \(N - 1\), where \(S_i\) and \(P_i\) are HRTMs

\[ S_i = S(\xi_i \sigma_i \sigma_{i+1} \xi_{i+1}) \]
\[ P_i = P(\eta_i+1 \sigma_{i+1} \sigma_i \eta_i) \].  
(3.2)

We have aligned the variables of HRTMs in the clockwise order as CTMs. At the moment all the HRTMs are equivalent, though we put indices for identification of their positions.

![Half-row transfer matrices between vectors L and R.](image)

We fix these \(N\) spins from the left to the right, successively calculating the conditional probability \(p_{\sigma_1, \ldots, \sigma_{i-1}}(\bar{\sigma}_i)\) for the spin at \(i\)-site after fixing those spins in the left \(\sigma_1, \ldots, \sigma_{i-1}\). The way of calculation is essentially the same as operator multiplication to a given matrix product state\(^3\) (MPS) in finite system DMRG algorithm, and it is numerically important to prepare partial sum of local factors in advance. We write \(R\) as \(R_N\) since it contains \(\sigma_N\) as its variable. Let us multiply the transfer matrices \(T_i\) one by one to the vector \(R_N\).

\[ R_{N-1} = T_{N-1} R_N \]
\[ R_{N-2} = T_{N-2} R_{N-1}, \text{ etc.} \]  
(3.3)

down to \(R_1\). In the numerical calculation we do not possess the transfer matrix \(T_i\) explicitly, but we apply \(S_i\) and \(P_i\) part by part as

\[ R(\eta, \sigma_1 \xi_1) = \sum_{\sigma_{i+1} \xi_{i+1}} S(\xi_i \sigma_i \sigma_{i+1} \xi_{i+1}) \]
\[ \sum_{\eta_{i+1}} R(\xi_{i+1} \sigma_{i+1} \eta_{i+1}) P(\eta_{i+1} \sigma_{i+1} \sigma_i \eta_i), \]  
(3.4)

where the second sum should be taken first. (See Fig. 5.)

Fig. 4. Half-row transfer matrices between vectors \(L\) and \(R\).  

After obtaining \(R_1\) we can calculate the probability for \(\sigma_1\) as before

\[ p(\bar{\sigma}_1) = \frac{|\langle L_1 | \delta(\bar{\sigma}_1, \sigma_1) | R_1 \rangle|^2}{\langle L_1 | R_1 \rangle}, \]  
(3.5)

where we have written \(L\) as \(L_1\) since it contains \(\sigma_1\) as its variable. According to this probability we stochastically fix the first spin in the row. We then consider the conditional probability \(p_{\bar{\sigma}_2}(\sigma_2)\) for the second spin after fixing the first one. This time, we have to prepare \(L_1\) multiplied by \(T\)

\[ L(\eta_2 \sigma_2 \xi_2) = \sum_{\eta_1} P(\eta_2 \sigma_2 \bar{\sigma}_1 \eta_1) L(\eta_1 \bar{\sigma}_1 \xi_1) S(\xi_1 \sigma_1 \sigma_2 \xi_2) \]  
(3.6)

as shown in Fig. 5. It should be noted that we do not take configuration sum for \(\sigma_1\) since it is already fixed; \(L_2\) contains a fixed spin \(\bar{\sigma}_1\) in it. Using \(R_2\) calculated before and \(L_2\) in Eq.(3.6), we obtain the conditional probability for the second spin

\[ p_{\bar{\sigma}_1}(\sigma_2) = \frac{|\langle L_2 | \delta(\bar{\sigma}_2, \sigma_2) | R_2 \rangle|^2}{\langle L_2 | R_2 \rangle}, \]  
(3.7)

According to this probability we can fix the second spin. After that we calculate \(L_3\) in the same manner as Eq.(3.6). Repeating these spin fixing procedure to \(\sigma_N\), we finally obtain a spin snapshot \(\{\bar{\sigma}\} = \bar{\sigma}_1, \bar{\sigma}_2, \ldots, \bar{\sigma}_N\) for a group of \(N\) spins in a row.

§4. Snapshot in a Rectangular Area

![The double-row spin system. The cross marks represent the already fixed spins in the first row, and the circles are those spins that we will fix each by each.](image)

Let us consider the way of fixing \(M\) numbers of spin rows successively. The first step is to obtain the probability for the second spin row under the condition that the first row \(\bar{\sigma}_1, \bar{\sigma}_2, \ldots, \bar{\sigma}_N\) is already fixed. For the distinction let us write the spins in the second row as \(\{\tau\} =\)
\(\tau_1, \tau_2, \ldots, \tau_N\). Figure 6 shows the system that we consider for a while, where there is a transfer matrix to the vertical direction between \(\{\sigma\}\) shown by cross marks and \(\{\tau\}\) by circles. This transfer matrix consists of the right HRTM \(O(\nu \bar{\sigma}_N \tau_N \nu')\), the left one \(Q(\mu' \tau_i \bar{\sigma}_i \mu)\), and \(N - 1\) numbers of local Boltzmann weights \(W(\tau_i, \bar{\sigma}_i, \bar{\sigma}_{i+1})\) from \(i = 1\) to \(N - 1\) in between. \(^8\)

We reduce the above double-row system to the single-row one treated in the previous section by way of extension of the CTMs and HRTMs to the vertical direction, similar to the system size extension in CTMRG. \(^7\) The HRTM \(S\) is extended by putting \(W\) on top of it

\[
S'(\xi_i, \tau_i, \tau_{i+1}, \bar{\xi}_{i+1}) = W(\tau_i, \tau_{i+1}, \bar{\sigma}_i, \bar{\sigma}_{i+1})S(\xi_i, \bar{\sigma}_i, \bar{\sigma}_{i+1}, \bar{\xi}_{i+1})
\]

as shown in Fig. 7. Here we do not regard \(\bar{\sigma}_i\) and \(\bar{\sigma}_{i+1}\) as the variable of the extended HRTM \(S'\) since these are fixed constants. Thus the number of elements in \(S'_i\) is the same as that of \(S_i\). It should be noted that after such an extension \(S'_i\) becomes position dependent.

![Fig. 7. Extension of the HRTM S to the vertical direction.](attachment:image)

The area extension of CTMs \(A\) and \(D\) are done by putting HRTMs \(Q\) and \(O\)

\[
A'(\xi_N, \tau_N, \nu) = \sum_{\nu} A(\xi_N, \bar{\sigma}_N, \nu)O(\nu \bar{\sigma}_N, \tau_N, \nu')
\]

\[
D'(\mu', \tau, \xi) = \sum_{\mu} Q(\mu', \tau, \bar{\sigma}_i, \mu)D(\mu, \mu, \bar{\sigma}_i, \xi)
\]

respectively, as shown in Fig. 8. Again, the number of elements in the extended CTMs are the same as the original ones. In this way we have reduced the double row system in Fig. 6 as single row one constructed from \(A', B, C, D', P_i\), and \(S'_i\). The spin fixing procedure from the left to right explained in the previous section is now applicable to the second row of spins \(\{\tau\}\). It is straightforward to repeat the extension of HRTMs and CTMs to the vertical direction for \(M - 1\) times, we finally obtain the snapshot of the size \(N \times M\) in the infinite system.

![Fig. 8. Area extension of CTMs D and A.](attachment:image)

§5. Conclusion and Discussion

We have explained the way of obtaining spin snapshot in the area of \(N \times M\) for the 2D Ising model. The snapshot observation can be applied to various 2D lattice systems and 1D quantum systems. The snapshot in the former corresponds to many time observation result in the latter. A snapshot can be regarded as a representative path in the path integral formulation of quantum systems. Successive observations in time-dependent DMRG\(^10,11\) for numbers of time slices is the same type of computation.

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