

A NOVEL METHOD FOR COMPUTING THE PARTITION FUNCTION OF MARKOV
RANDOM FIELD IMAGES USING MONTE CARLO SIMULATIONS

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ABSTRACT

We show that the partition function of a general Markov random field is equivalent to an expectation. This observation allows the development of an importance sampling procedure to estimating this expectation by using Monte-Carlo simulations.

I. INTRODUCTION

Markov random fields (MRF's) belong to a well known and popular class of parametric random field models. They are extensively used for modeling spatial interaction phenomena. However, many theoretical and computational difficulties prohibit the application of these models to a wide class of problems, one of the major difficulties being the computation of the *partition function*. No exact solutions are known for this problem, except for very simple cases [1], which are not adequate for most applications of interest.

The lack of a closed form solution for the partition function imposes many restrictions. For example, the statistical inference of MRF's, via a maximum likelihood approach, is an open problem, since solution of the likelihood equations is impossible without knowing the exact value of the partition function. It is, therefore, clear that the problem of calculating the partition function of a general MRF is important. The study of this problem is the purpose of the present paper.

II. MARKOV RANDOM FIELDS

Assume that we have a collection of $M \times N$ sites which form a two-dimensional rectangular lattice $\Lambda_{MN} = \{(i, j) : 1 \leq i \leq M, 1 \leq j \leq N\}$. A discrete random variable $H(i, j)$ is assigned at each site of the lattice, taking values from an ensemble $E_H = \{\phi_1, \phi_2, \dots, \phi_R\}$, which contains $R \geq 2$ distinct values. The resulting random field $[H] = \{H(i, j) : 1 \leq i \leq M, 1 \leq j \leq N\}$ can take any one of the R^{MN} possible realizations $[h] = \{h_{ij} : 1 \leq i \leq M, 1 \leq j \leq N\}$ in the Cartesian product E_H^{MN} with joint probability distribution $Pr[H=h]$. We shall restrict $[H]$ to be in the class of MRF's, whose joint probability distribution is given by the Gibbs measure

$$Pr[H=h] = \frac{1}{Z_{MN}} \prod_{i=1}^M \prod_{j=1}^N \sigma_{ij}(h_{ij}, h_{i-1,j}, h_{i-1,j-1}, h_{i,j-1}), \quad (1a)$$

where

$$Z_{MN} = \sum_{\text{states } h} \prod_{i=1}^M \prod_{j=1}^N \sigma_{ij}(h_{ij}, h_{i-1,j}, h_{i-1,j-1}, h_{i,j-1}). \quad (1b)$$

In (1), Z_{MN} is a normalizing constant known as the *partition function*, whereas, $\sigma_{ij}(x, y, z, \omega)$ is the *local transfer function* (LTF) of the MRF $[H]$ [2]. The LTF is a function of a positive parameter T , known as the *temperature*, which controls the degree of peaking in the Gibbs measure.

A special case of a general MRF is a *mutually compatible Gibbs random field* (MC-GRF) [2]. The probability structure of a subset $[H]_A$ of such a random field $[H]$, restricted on a finite sublattice A of Λ_{MN} , is independent of the size, or shape, of A . The LTF $\tau_{ij}(x, y, z, \omega)$ of these MRF's is restricted to satisfy the following relationship:

$$\sum_{u \in E_H} \tau_{ij}(u, y, z, \omega) = k_{ij},$$

for every triplet $(y, z, \omega) \in E_H^3$, where k_{ij} is a constant. Generating a realization of a MC-GRF is an easy task, because this can be done lexicographically using point by point simulation, as the following relation implies:

$$\begin{aligned} Pr[H=h] &= \prod_{i=1}^M \prod_{j=1}^N \frac{\tau_{ij}(h_{ij}, h_{i-1,j}, h_{i-1,j-1}, h_{i,j-1})}{\sum_{u \in E_H} \tau_{ij}(u, h_{i-1,j}, h_{i-1,j-1}, h_{i,j-1})} \\ &= \prod_{i=1}^M \prod_{j=1}^N Pr[h_{ij} | h_{i-1,j}, h_{i-1,j-1}, h_{i,j-1}]. \end{aligned}$$

Therefore, knowing the values of random variables $H(i-1, j)$, $H(i-1, j-1)$ and $H(i, j-1)$, we can generate the value of $H(i, j)$ by sampling the conditional probability $Pr[h_{ij} | h_{i-1,j}, h_{i-1,j-1}, h_{i,j-1}]$ over all possible values in E_H .

III. MONTE-CARLO CALCULATION OF THE
PARTITION FUNCTION

Assume that $P_{MN}(h)$ is a joint probability distribution defined on the space of all R^{MN} realizations h . In this case

$$Z_{MN} = \sum_{\text{states } h} \left[\frac{A_{MN}(h)}{P_{MN}(h)} \right] P_{MN}(h), \quad (2a)$$

where

$$A_{MN}(h) = \prod_{i=1}^M \prod_{j=1}^N \sigma_{ij}(h_{ij}, h_{i-1,j}, h_{i-1,j-1}, h_{i,j-1}). \quad (2b)$$

From (2) we derive the following estimate \hat{Z}_{MN} for the partition function Z_{MN} :

$$\hat{Z}_{MN} = \lim_{K \rightarrow +\infty} \hat{Z}_{MN}(K) = \lim_{K \rightarrow +\infty} \left[\frac{1}{K} \sum_{i=1}^K \frac{A_{MN}(h_i)}{P_{MN}(h_i)} \right], \quad (3a)$$

provided that

$$\frac{A_{MN}(h)}{P_{MN}(h)} < +\infty, \quad (3b)$$

for every $h \in E_H^{MN}$. In (3), h_i , $i = 1, 2, \dots, K$, are realizations drawn with probability $P_{MN}(h_i)$, and, therefore, \hat{Z}_{MN} is a Monte-Carlo estimate of the partition function [3]. Inequality (3b) is usually satisfied in the case of small lattices. When $M, N \rightarrow +\infty$, this inequality may be violated and our approach has to be modified. This modification will be discussed shortly.

Since $\hat{Z}_{MN}(K)$, and, therefore, \hat{Z}_{MN} , are unbiased estimators of Z_{MN} [3], we shall concentrate on finding joint probability distributions $P_{MN}(h)$ which result in a small error variance $E_P[(\hat{Z}_{MN}(K) - Z_{MN})^2]$, for every K . Consider probability distributions $P_{MN}(h)$ which correspond to a MC-GRF, therefore, satisfying the following relation:

$$P_{MN}(h) = \prod_{i=1}^M \prod_{j=1}^N \tau_{ij}(h_{ij}, h_{i-1,j}, h_{i,j-1}, h_{i,j-1}) > 0, \quad (4a)$$

where

$$\sum_{u \in E_H} \tau_{ij}(u, y, z, \omega) = 1, \quad \text{for every } (y, z, \omega) \in E_H^3. \quad (4b)$$

This is a convenient choice, since drawing samples from $P_{MN}(h)$ (i.e., generating a realization of a MC-GRF) is an easy task, as it was mentioned in the previous section. Computing the ratio $A_{MN}(h)/P_{MN}(h)$ is also straightforward. Indeed, if

$$q_{ij}(h_{ij}, h_{i-1,j}, h_{i,j-1}, h_{i,j-1}) = \frac{\sigma_{ij}(h_{ij}, h_{i-1,j}, h_{i,j-1}, h_{i,j-1})}{\tau_{ij}(h_{ij}, h_{i-1,j}, h_{i,j-1}, h_{i,j-1})}, \quad (5a)$$

and

$$Q_{MN}(h) = \prod_{i=1}^M \prod_{j=1}^N q_{ij}(h_{ij}, h_{i-1,j}, h_{i,j-1}, h_{i,j-1}), \quad (5b)$$

then (see (2), (4) and (5))

$$Z_{MN} = \sum_{\text{states } h} Q_{MN}(h) P_{MN}(h), \quad (6)$$

and

$$\hat{Z}_{MN} = \lim_{K \rightarrow +\infty} \hat{Z}_{MN}(K) = \lim_{K \rightarrow +\infty} \left[\frac{1}{K} \sum_{i=1}^K Q_{MN}(h_i) \right], \quad (7a)$$

provided that

$$Q_{MN}(h) < +\infty, \quad (7b)$$

for every $h \in E_H^{MN}$.

A simple choice for the LTF of a MC-GRF could be $\tau_{ij}(x, y, z, \omega) = 1/R$, for every $(x, y, z, \omega) \in E_H^4$ and every $(i, j) \in \Lambda_{MN}$. In this case $P_{MN}(h) = 1/R^{MN}$ (i.e., the joint probability distribution of an i.i.d. random field). In most practical situations one does not expect the i.i.d. choice to give a good estimate of Z_{MN} in a reasonable time. The reason for this is that, in most cases of interest (e.g., in low temperatures), only a small fraction of realizations h_i contribute to the partition function sum, while the contribution of most other realizations is negligible.

If we now choose the joint probability distribution of a MC-GRF which is "as close as possible" to the Gibbs measure, then this choice will favor the most probable realizations of the MRF over the less probable ones. This will result in a reduction of the error variance. It is now natural to seek the optimal joint probability distribution $P_{MN}^{opt}(h)$ of a MC-GRF, by solving the following constrained minimization problem:

$$P_{MN}^{opt}(h) = \arg \{ \min_P \text{Var}_P[\hat{Z}_{MN}(K)] \}, \quad \text{such that (4) holds.}$$

However, the solution of this problem is not feasible in general. Therefore, we shall derive a *suboptimal* solution. We have the following theorem.

Theorem: For every joint probability distribution $P_{MN}^{(1)}(h)$, satisfying (4), there will be a joint probability distribution $P_{MN}^{(2)}(h)$, satisfying (4), with

$$\tau_{ij}^{(2)}(x, y, z, \omega) = \tau_{ij}^{(1)}(x, y, z, \omega),$$

for every $(i, j) \in \Lambda_{MN} - \{(M, N)\}$ and

$$\tau_{MN}^{(2)}(x, y, z, \omega) = \frac{\sigma_{MN}(x, y, z, \omega)}{\sum_{u \in E_H} \sigma_{MN}(u, y, z, \omega)},$$

for every $(x, y, z, \omega) \in E_H^4$, such that

$$\text{Var}_{P \circ \omega}[\hat{Z}_{MN}(K)] \leq \text{Var}_P[\hat{Z}_{MN}(K)].$$

Given the LTF $\sigma_{ij}(x, y, z, \omega)$ of a MRF, our suboptimal choice for the joint probability distribution $P_{MN}(h)$ will be a joint probability distribution $P_{MN}^*(h)$, given by (4), with LTF

$$\tau_{ij}^*(x, y, z, \omega) = \frac{\sigma_{ij}(x, y, z, \omega)}{\sum_{u \in E_H} \sigma_{ij}(u, y, z, \omega)}, \quad (8)$$

for every $(x, y, z, \omega) \in E_H^4$ and every $(i, j) \in \Lambda_{MN}$.

The MC-GRF with LTF given by (8) corresponds to the MC-GRF obtained by approximating a general MRF via the "Approach B" developed in [4]. This is a sensible choice, because the computation of the joint probability distribution $P_{MN}^*(h)$ is feasible, and the obtained MC-GRF contains substantial information about the original MRF [4], much more than the i.i.d. random field, which contains absolutely no information about the MRF in low temperatures.

After deciding for the choice of the MC-GRF joint probability distribution to be used in the Monte-Carlo partition function calculation, the next step is to determine how to implement this calculation in a computationally efficient way. A simple approach is to use the following algorithm (which is based on the *Gibbs sampler* described in [5]):

ALGORITHM:

1. Generate a realization h_1 of the MC-GRF with probability $P_{MN}^*(h)$, given by (4), with $\tau_{ij}(x, y, z, \omega) = \tau_{ij}^*(x, y, z, \omega)$, given by (8). This is done lexicographically. Calculate $Q_{MN}(h_1)$, given by (5), with $\tau_{ij}(x, y, z, \omega) = \tau_{ij}^*(x, y, z, \omega)$, given by (8).
2. Set $SUM = QFUN = Q_{MN}(h_1)$ and $m = 1$.
3. Select a site $(i, j) \in \Lambda_{MN}$ randomly, with probability $1/MN$ among all sites in Λ_{MN} and set $s = h_{ij}^{(m)}$.
4. Draw a value ϕ_k from probability $d_k / (\sum_{i=1}^R d_i)$, where

$$d_i = \tau_{ij}^*(\phi_i, h_{i-1,j}^{(m)}, h_{i-1,j-1}^{(m)}, h_{i,j-1}^{(m)}) \tau_{i+1,j}^*(h_{i+1,j}^{(m)}, h_{i-1,j+1}^{(m)}, h_{i-1,j}^{(m)}, \phi_i) \\ \times \tau_{i+1,j}^*(h_{i+1,j}^{(m)}, \phi_i, h_{i,j-1}^{(m)}, h_{i+1,j-1}^{(m)}) \tau_{i+1,j+1}^*(h_{i+1,j+1}^{(m)}, h_{i,j+1}^{(m)}, \phi_i, h_{i+1,j}^{(m)}).$$

5. If $\phi_k = s$ go to step 6, otherwise compute the ratio

$$RATIO = Q_{MN}(h_{m+1}) / Q_{MN}(h_m),$$

by

RATIO =

$$= \frac{q_{ij}(\phi_k, h_{i-1,j}^{(m)}, h_{i-1,j-1}^{(m)}, h_{i,j-1}^{(m)}) q_{i,j+1}(h_{i,j+1}^{(m)}, h_{i-1,j+1}^{(m)}, h_{i-1,j}^{(m)}, \phi_k)}{q_{ij}(s, h_{i-1,j}^{(m)}, h_{i-1,j-1}^{(m)}, h_{i,j-1}^{(m)}) q_{i,j+1}(h_{i,j+1}^{(m)}, h_{i-1,j+1}^{(m)}, h_{i-1,j}^{(m)}, s)} \\ \frac{q_{i+1,j}(h_{i+1,j}^{(m)}, \phi_k, h_{i,j-1}^{(m)}, h_{i+1,j-1}^{(m)}) q_{i+1,j+1}(h_{i+1,j+1}^{(m)}, h_{i,j+1}^{(m)}, \phi_k, h_{i+1,j}^{(m)})}{q_{i+1,j}(h_{i+1,j}^{(m)}, s, h_{i,j-1}^{(m)}, h_{i+1,j-1}^{(m)}) q_{i+1,j+1}(h_{i+1,j+1}^{(m)}, h_{i,j+1}^{(m)}, s, h_{i+1,j}^{(m)})},$$

where $q_{ij}(x, y, z, \omega)$ is given by (5a), with $\tau_{ij}(x, y, z, \omega) = \tau_{ij}^*(x, y, z, \omega)$, given by (8). Set $QFUN \leftarrow QFUN \times RATIO$.

6. Set $SUM \leftarrow SUM + QFUN$. If $m + 1 = K$, set $\hat{Z}_{MN}(K) = SUM / (m + 1)$ and stop; otherwise, set $h_{ij}^{(m+1)} = \phi_k$, $h_k^{(m+1)} = h_k^{(m)}$, for every $(k, l) \neq (i, j)$, $m \leftarrow m + 1$, and go to step 3.

We are now interested in the statistical properties of the estimator $\hat{Z}_{MN}(K)$, resulting from our *Algorithm*. The estimator $\hat{Z}_{MN}(K)$ is the sum of identically distributed random variables $Q_{MN}(h_i)$, which are characterized by a finite mean $\mu_{MN} = Z_{MN}$ and finite, nonzero variance σ_{MN}^2 . Obviously, $\hat{Z}_{MN}(K)$ is an unbiased estimator of Z_{MN} . The computation of the variance of $\hat{Z}_{MN}(K)$ requires more effort. We can easily show that [6]

$$KVar_p[\hat{Z}_{MN}(K)] =$$

$$= Q^T \left[P^* - P^* A + 2 P^* \sum_{l=1}^{K-1} \frac{K-l}{K} (P^l - A) \right] Q, \quad (9)$$

where all the matrices are $R^{MN} \times R^{MN}$ matrices. Matrix P^* is a diagonal matrix with elements the R^{MN} probabilities $P_{MN}^*(h)$, $h \in E_H^{MN}$. Matrix A has R^{MN} identical rows which are equal to the diagonal of P^* , whereas, P^l is the l power of the transition probability matrix P . Finally, Q is an R^{MN} -dimensional vector, with elements $Q_{MN}(h)$, $h \in E_H^{MN}$. For an ergodic transition probability matrix P the *fundamental matrix* F , given by $F = (I - P + A)^{-1}$, exists, and

$$F = I + \lim_{K \rightarrow +\infty} \sum_{l=1}^{K-1} \frac{K-l}{K} (P^l - A). \quad (10)$$

From (9) and (10) we obtain

$$\lim_{K \rightarrow +\infty} KVar_p[\hat{Z}_{MN}(K)] = Q^T \left[2P^*F - P^* - P^*A \right] Q,$$

or

$$\lim_{K \rightarrow +\infty} Var_p[\hat{Z}_{MN}(K)] = 0. \quad (11)$$

From (11) and the *Tchebycheff inequality* we can easily show that our *Algorithm* results in an unbiased, consistent and asymptotically efficient estimator for Z_{MN} .

In many instances $Z_{MN} \rightarrow +\infty$ with increasing lattice size (i.e., as $M, N \rightarrow +\infty$). Additionally, for many realizations h , $P_{MN}(h) \rightarrow 0$, whereas, $A_{MN}(h) \rightarrow +\infty$ as $M, N \rightarrow +\infty$.

Therefore, (3b) may be violated. Since most applications require use of rather large lattices, we have to examine the problems introduced by this behavior and modify our Monte-Carlo calculation procedure. It is clear that, in these cases our *Algorithm* will suffer from *overflow* problems.

To overcome this problem define

$$f(Z_{MN}) = \frac{1}{MN} \ln(Z_{MN}).$$

Observe now that

$$f(Z_{MN}) = \frac{1}{MN} \ln \left[\sum_{states \ h} Q_{MN}(h) P_{MN}(h) \right] \\ = \ln q_{\max} + \frac{1}{MN} \ln \left[\sum_{states \ h} Q'_{MN}(h) P_{MN}(h) \right], \quad (12)$$

where

$$q_{ij}^{(max)} = \max_{(x,y,z,\omega) \in E_H^4} \left[q_{ij}(x,y,z,\omega) \right],$$

$$q_{\max} = \left[\prod_{i=1}^M \prod_{j=1}^N q_{ij}^{(max)} \right]^{\frac{1}{MN}},$$

and

$$Q'_{MN}(h) = \prod_{i=1}^M \prod_{j=1}^N \frac{q_{ij}(h_{ij}, h_{i-1,j}, h_{i-1,j-1}, h_{i,j-1})}{q_{ij}^{(max)}}.$$

From (12) we see that, in order to compute $f(Z_{MN})$ we have to calculate the expectation $E_P[Q'_{MN}(h)]$. This can be done by a simple modification of our *Algorithm*. Notice that, in this case, Monte-Carlo calculations can proceed with no overflow, even in the case of large lattices, because $Q'_{MN}(h) \leq 1 < +\infty$, for all realizations h ; therefore, condition (3b), or (7b), is satisfied. Equation (12) yields the following Monte-Carlo estimate for $f(Z_{MN})$

$$\hat{f}_K(Z_{MN}) =$$

$$= \frac{1}{MN} \ln(\hat{Z}_{MN}(K)) = \ln q_{\max} + \frac{1}{MN} \ln \left[\frac{1}{K} \sum_{i=1}^K Q'_{MN}(h_i) \right],$$

where h_i are samples drawn from the joint probability distribution $P_{MN}^*(h)$.

It is worthwhile noticing that the estimator $\ln(\hat{Z}_{MN}(K))$ will only asymptotically (i.e., for $K \rightarrow +\infty$) yield an unbiased and efficient estimate for $\ln(Z_{MN})$ [6]. Finally, we can easily show that $\ln(\hat{Z}_{MN}(K))$ is a consistent estimator for $\ln(Z_{MN})$.

IV. SIMULATION EXPERIMENTS

So far we have demonstrated the fact that the partition function of a general MRF can be effectively calculated by using the Monte-Carlo scheme discussed. A major question to be answered is how well the proposed algorithm works. We shall examine this question by comparing simulated results with available analytical results [7], [8]. We consider a special MRF, the two-dimensional Ising model with no external magnetic field and nearest neighbor interactions, defined on a rectangular lattice with toroidal boundary conditions. For such a MRF $R=2$, $E_H = \{-1, +1\}$ and

$$\sigma(x, y, z, \omega) = \exp \left[\frac{1}{T} (Bxy + A\omega) \right].$$

This model exhibits phase transition at a *critical temperature* T_c , at which the *internal energy per site* $E_{MN}(T) = T^2/MN \partial \ln Z_{MN} / \partial T$ is discontinuous, and the *specific heat* $C_{MN}(T) = \partial E_{MN}(T) / \partial T$ is infinite, as $M, N \rightarrow +\infty$ [7].

In our simulation experiments, estimates of $f(Z_{MN})$, $E_{MN}(T)$ and $C_{MN}(T)$ (see [6] for details), for a variety of parameters A, B, T , and lattice sizes, have been obtained using our *Algorithm*. The comparison with available analytical results shows that our method gives accurate results within a reasonable number of iterations. As, however, the lattice size increases, more iterations are necessary, especially around the critical temperature. Some preliminary results are given in Table I, for a 16×16 site Ising model, with $A=B=1.0$, at various temperatures. A typical convergence behavior of our algorithm, estimating $\ln(Z_{MN})$ is depicted in Fig. 1, for the same Ising model at $T=3.0$. Finally, estimated curves of $\hat{f}(Z_{MN})$, $\hat{E}_{MN}(T)$ and $\hat{C}_{MN}(T)$ of an 8×8 site Ising model (with $A=B=1.0$) are given in Fig. 2. The peak of the specific heat curve occurs at $\hat{T}_c = 2.4$, which is very close to the actual value $T_c = 2.269$.

Other simulation experiments, based on more general MRF's, have been carried out with extremely encouraging results. This shows that our method works well.

V. CONCLUSION

We have presented a new Monte-Carlo simulation technique for the estimation of the partition function of a general MRF, which results in unbiased, consistent and asymptotically efficient estimates. This technique gives extremely accurate results, as demonstrated by our simulations. Use of more efficient algorithms can boost the performance and accuracy of the method, and yield more reliable estimates.

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ISING MODEL, 16×16 sites, $A=1.0, B=1.0, T_c=2.27$						
T	$f(Z_{MN})$		$-E_{MN}(T)$		$C_{MN}(T)$	
	EST.	EXACT	EST.	EXACT	EST.	EXACT
5.00	0.7345	0.7345	0.4274	0.4282	0.10	0.09
4.00	0.7591	0.7591	0.5560	0.5573	0.17	0.17
3.00	0.8159	0.8159	0.8120	0.8173	0.37	0.40
2.27	0.9346	0.9319	1.2011	1.4129	0.44	1.64
2.00	1.0127	1.0289	1.4717	1.7440	0.35	0.73
1.00	2.0025	2.0003	1.9970	1.9972	0.02	0.02
0.50	4.0027	4.0027	2.0000	2.0000	0.00	0.00

Table I: Comparison of exact and estimated quantities for the Ising model.

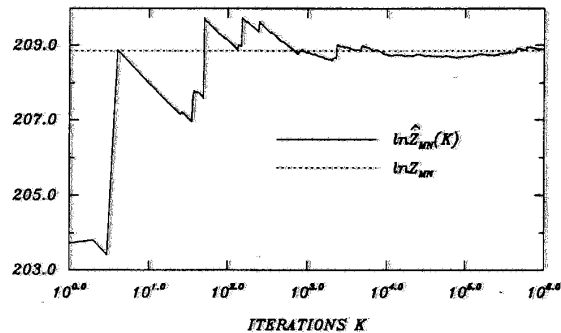


Figure 1: Convergence behavior of $\ln(Z_{MN})$ for a 16×16 site Ising model ($A=B=1.0, T=3.0$).

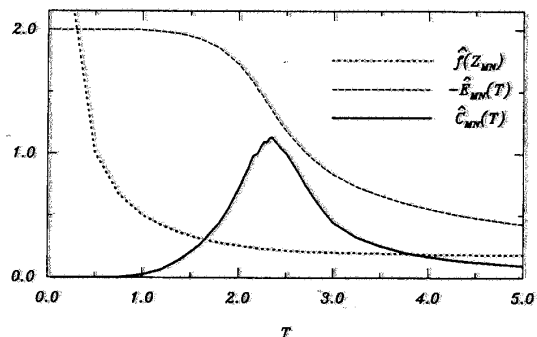


Figure 2: Estimated curves of $\hat{f}(Z_{MN})$, $\hat{E}_{MN}(T)$ and $\hat{C}_{MN}(T)$ for an 8×8 site Ising model ($A=B=1.0$).