Theoretical and computational aspects of 1-vertex transfer matrices

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Abstract

We introduce the notion of 1-vertex transfer matrix for near neighbor Potts models with k kinds of particles. We show that the topological entropy (free energy) of this model can be expressed as the limit the logarithm of spectral radii of 1-vertex transfer matrices. Storage and computations using the 1-vertex transfer matrix are much smaller than storage and computations needed for the standard transfer matrix that is used. We apply our methods to find at least the first 15 digits of the entropy of the hard core model on the two dimensional integer grid.

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1 Statements of the results

In many models of statistical mechanics one uses Potts models, which can be considered as coloring the lattice $\mathbb{Z}^d$ in k colors, with some local restrictions on the coloring. In this paper we assume that the coloring conditions are *symmetric* and *isotropic*: Let $\Delta = (V, E), V = \{1, \ldots, k\}$ be an undirected graph on k vertices, where vertex i is identified with the color i. Then two neighboring points $\mathbf{p} = (p_1, \ldots, p_d)^\top, \mathbf{q} = (q_1, \ldots, q_d) \in \mathbb{Z}^d$, i.e. $\sum_{l=1}^d |p_i - q_i| = 1$, can be colored in colors $i, j \in V$ if and only if $(i, j) \in E$. We assume that Δ is a connected graph.

For any $X \subseteq \mathbb{Z}^d$ let $\mathrm{C}_\Delta(\mathrm{X})$ be the set of all possible coloring in k colors, subject to the restrictions given by the graph Δ. View $\alpha \in \mathrm{C}_\Delta(\mathrm{X})$ as a map $\alpha : X \to \{1, \ldots, k\}$. Let $\mathbb{N}$ be the set of positive integers and for $m \in \mathbb{N}$ let $\langle m \rangle := \{1, \ldots, m\} \subset \mathbb{N}$. For $\mathbf{p} = (p_1, \ldots, p_d)^\top \in \mathbb{N}^d$ we let $\langle \mathbf{p} \rangle := \langle p_1 \rangle \times \ldots \times \langle p_d \rangle \subset \mathbb{N}^d$ be a box of lattice points of dimensions $p_1 \times \ldots \times p_d$. For $m, d \in \mathbb{N}$ let $\mathbf{m}_d := (m, \ldots, m) \in \mathbb{N}^d$.

The physical quantities that are of interest are obtained as a limit of the corresponding quantities, which depend on the allowable colorings in the cube $\langle \mathbf{m}_d \rangle$. One of the main theoretical and computational concepts in statistical mechanics is the concept of the *transfer matrix*. For $d \geq 2$ the transfer matrix is given by $T_{m,d} = [t_{\alpha\beta,m,d}] \in \{0,1\}^{N_{m,d} \times N_{m,d}}$, where $\alpha, \beta \in \mathrm{C}_\Delta(\langle \mathbf{m}_{\mathrm{d}-1} \rangle)$ are allowable coloring of the $d-1$ dimensional cube $\langle \mathbf{m}_{d-1} \rangle$ and $N_{m,d} := \#\mathrm{C}_\Delta(\langle \mathbf{m}_{\mathrm{d}-1} \rangle)$. $t_{\alpha\beta,m,d}$ is equal to 1 or 0 if the coloring of the box $\langle \mathbf{m}_{d-1} \rangle \times \langle 2 \rangle \subset \mathbb{N}^d$ by the colors α and β on the sets $\langle \mathbf{m}_{d-1} \rangle \times \{1\}$ and $\langle \mathbf{m}_{d-1} \rangle \times \{2\}$ respectively is Δ allowed or forbidden coloring. (For $d = 1$ we can only choose $m = 1$, and $T_{1,1}$ is the incidence matrix of Δ.) Note that $T_{m,d}$ is symmetric.

By considering the allowable coloring of the infinite strip $\langle \mathbf{m}_{d-1} \rangle \times \mathbb{Z} \subset \mathbb{Z}^d$, we obtain that the physical quantities depend on the matrix $T_{m,d}$, e.g. its spectral radius $\rho(T_{m,d})$.

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See the detailed description of this approach in [3]. In order to obtain good evaluations of physical concepts one needs to choose m sufficiently big. Usually, $N_{m,d}$ is of order $c^{m^{d-1}}$, which means in the reality of computations one has to choose m relatively small. Note that for $d = 1$ the computations depend only on the $k \times k$ adjacency matrix of Δ, which we assume to be trivial. Thus we assume the nontrivial case $d \geq 2$.

The purpose of this paper to introduce the notion of 1-vertex transfer matrix for $d \geq 2$. This matrix denoted by $S_{m,d} = [s_{\alpha\beta,m,d}] \in \{0,1\}^{M_{m,d}\times M_{m,d}}$, where $M_{m,d} \leq N_{m,d}$. $\alpha, \beta \in \mathrm{C}_\Delta(\widehat{\langle \mathbf{m}_{\mathrm{d}-1}\rangle}) \subseteq \mathrm{C}_\Delta(\langle \mathbf{m}_{\mathrm{d}-1}\rangle)$. If $s_{\alpha\beta,m,d} = 1$, then coloring of α and β are closely related. Namely, given the coloring α or β one knows the coloring of β or α respectively, except at most in one lattice point. The numerical advantage of $S_{m,d}$ is that it is a very sparse matrix. Hence the storage and the computations using the 1-vertex transfer matrix are much smaller than storage and computations needed for the standard transfer matrix $T_{m,d}$. More precisely the number of nonzero elements in each row of $S_{m,d}$ is at most k. However $S_{m,d}$ is not a symmetric matrix. Let $S^{\ell}_{m,d} = [s^{(\ell)}_{\alpha\beta,m,d}]$ for $\ell \in \mathbb{N}$. We show that $s^{(m^{d-1})}_{\alpha\beta,m,d} \leq t_{\alpha\beta,m,d}$ for all $\alpha, \beta \in \mathrm{C}_\Delta(\widehat{\langle \mathbf{m}_{\mathrm{d}-1}\rangle})$. Hence $\rho(S_{m,d})^{m^{d-1}} \leq \rho(T_{m,d})$. It can be shown the physical quantities that one wants to compute can be the expressed in terms of $S_{m,d}$.

To illustrate this claim we consider the topological entropy of the coloring of $\mathbb{Z}^d$ given by Δ. This is the limit of the logarithm of all allowable coloring of the cube $\langle \mathbf{m}_d \rangle$ divided by m^d as $m \to \infty$. This limit is also equal to $h_d(\Delta) := \lim_{m\to\infty} \frac{\log \rho(T_{m,d})}{m^{d-1}}$. See for example [3]. In this paper we show that $h_d(\Delta) = \lim_{m\to\infty} \log \rho(S_{m,d})$. In computations $h_d(\Delta)$ is approximated by $\frac{\log \rho(T_{m,d})}{m^{d-1}}$. Actually it is known that $h_d(\Delta) \leq \frac{\log \rho(T_{m,d})}{m^{d-1}}, m = 2, \ldots$ See [2] or [3], which also give lower bounds. For $d = 2$ we show the inequalities

$$h_2(\Delta) \leq \frac{2k+1}{2k} \log \rho(S_{2k+1,2}) \leq \frac{\log \rho(T_{2k+1,2})}{2k} \quad k = 1, \ldots, \tag{1.1}$$

However the numerical computation of the sequence $\rho(S_{m,2}), m = 2, \ldots, M$ do not give good upper and lower bounds as in the case of the computation of $\frac{\rho(T_{m,2})}{m}, m = 2, \ldots, M$ [2].

We implement the above results to the *the hard core model* on $\mathbb{Z}^2$. This model corresponds to coloring of $\mathbb{Z}^2$ in two colors: black and white, where no two black colors are adjacent. (So $\Delta = (V = \{1,2\}, E = \{(1,2),(2,2)\}$.) The topological entropy $h_2(\Delta)$ of the hard core model is known within the precision of 10 digits precisely [5] and heuristically to 43 digits [1].

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